Gauge Fields, Mode Mixing and Local Density of States in a Quantum Point Contact

S. Ulreich and W. Zwerger

Sektion Physik, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 München, Germany

PACS. 03.80+r – General theory of scattering.
PACS. 72.10−d – Theory of electronic transport; scattering mechanisms.

Abstract. – It is shown that the elimination of the discrete transverse motion in a waveguide of arbitrary shape may be described in terms of a non-abelian gauge field for the longitudinal dynamics. This allows for an exact treatment of the scattering between different modes by eliminating the gauge field at the expense of a non-diagonal matrix of local subband energies. The method is applied to calculate the local density of states (LDOS) in a quantum point contact. Contrary to the total conductance which is well described by an adiabatic approximation, mode mixing turns out to play a crucial role for local properties like the LDOS.

The discovery of quantized longitudinal conductances in quantum point contacts created in a two-dimensional ballistic electron gas has launched a great number of theoretical papers dealing with quantum mechanical scattering in waveguides with a general wide-narrow-wide type geometry. Precise numerical calculations of the transmission amplitudes $t_{mn}$ between the transverse modes $m$ and $n$ in such a structure have shown that the adiabatic approximation $t_{mn} \sim \delta_{mn}$ – while not exact – works extremely well for the linear conductance

$$G = \frac{2e^2}{h} \sum_{nm} |t_{nm}|^2$$

of the point contact at zero temperature. The effect of scattering between different transverse modes is therefore negligible for the conductance, thus justifying the adiabatic approximations used in the early explanations of the observed quantization of $G$. In our present work, we develop a novel method dealing with quantum mechanical scattering in waveguides of arbitrary width. It is based on a gauge theoretic description of the effect of transverse modes on the dynamics of the longitudinal motion, which allows for an exact treatment of intersubband scattering. Using this formalism and the recursive Green function method, we calculate the local density of states in a quantum point contact. In the vicinity of the constriction this local property is strongly affected by the scattering between different transverse modes.

We consider a general wave guide in two dimensions with an arbitrary but fixed confining potential $V(x,y)$. To determine the exact scattering wave functions of the stationary
Schrödinger equation

\[
\left[-\frac{\hbar^2}{2M}\nabla^2 + V(x,y)\right] \psi(x,y) = E\psi(x,y)
\]

we first split off the discrete motion in the transverse coordinate \( y \). Quite generally, for any confining potential \( V(x,y) \) which approaches infinity as \( y \to \pm \infty \), the one-dimensional Schrödinger equation for the transverse motion has a complete and discrete basis of eigenstates \( \Phi_n^x(y) \) for every value of the longitudinal coordinate \( x \). These eigenstates and eigenenergies are of course position dependent. The position dependent eigenenergies \( \varepsilon_n(x) \) give rise to potential barriers for the electrons traversing the wave guide structure in longitudinal direction. The corresponding eigenfunctions can be chosen real globally, which is always possible in the absence of a magnetic field. The completeness of the transverse basis allows one to expand the total wave function in the form \( \psi(x,y) = \sum_n \chi_n(x)\Phi_n^x(y) \). Inserting this ansatz into the two-dimensional Schrödinger equation, we obtain

\[
\left[ \frac{\hat{p}^2}{2M} - i\hbar \frac{\partial}{\partial y} A(x)\hat{p} - \frac{\hbar^2}{2M} B(x) + \varepsilon(x) \right] \chi(x) = E\chi(x).
\]

Here \( \chi(x) = (\chi_1(x), \chi_2(x), \ldots) \) is the vector of the longitudinal wave functions for the different transverse eigenstates \( n \) and \( \hat{p} = -i\hbar\partial_x \) is the momentum operator for the longitudinal motion. To simplify the notation we have introduced the following matrices

\[
A_{nm}(x) := \int_{-\infty}^{+\infty} dy \Phi^x_n(y) \cdot \frac{\partial \Phi^x_m(y)}{\partial x} \quad \text{and} \quad B_{nm}(x) := \int_{-\infty}^{+\infty} dy \Phi^x_n(y) \cdot \frac{\partial^2 \Phi^x_m(y)}{\partial x^2}
\]

and also the diagonal matrix of the local subband energies

\[
\varepsilon_{nm}(x) := \langle n(x) | -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial y^2} + V(x,y)|m(x) \rangle = \varepsilon_n(x) \cdot \delta_{nm}.
\]

It is straightforward to see that \( A \) is antisymmetric, since the wave functions are real valued everywhere. Obviously \( A(x) \) and \( B(x) \) are smooth for confining potentials, which are smooth functions of the longitudinal coordinate \( x \). If there are regions in the form of an ideal lead, we have \( A(x) = B(x) = 0 \) and the above system decouples trivially.

A simple calculation leads to the following relation between the matrices \( A(x) \) and \( B(x) \)

\[
B(x) = \frac{dA(x)}{dx} + A^2(x),
\]

which was first discovered by Kuperin et al. [7]. This relation allows one to rewrite eq. (8) in the form

\[
\left[ \frac{1}{2M} (\hat{p} - i\hbar A(x))^2 + \varepsilon(x) \right] \chi(x) = E\chi(x).
\]

Formally this is an tensorial Hamilton operator acting on an infinite-dimensional vector of wave functions. Apparently, the form of our Hamiltonian now resembles the quantum mechanical Hamiltonian of a charged particle in a magnetic field, however, in the present case the gauge field \( A \) is a tensor instead of a vector.

We now consider unitary transformations performed on the set of transverse eigenfunctions, i.e. we introduce a local gauge transformation (the bar denotes complex conjugation)

\[
\bar{k}(x) = \sum_n \bar{S}_{kn}(x)n(x),
\]
which mixes the different transverse eigenmodes. Since we do not want to change the physics via this operation, we also have to change our longitudinal coefficients according to

$$\tilde{\chi}_k(x) = \sum_l S_{kl}(x)\chi_l(x),$$

leaving the entire wave function invariant. It is straightforward to show, how the differential equation (7) for the longitudinal coefficients changes under this transformation. The transformation law for the diagonal matrix of subband energies $\varepsilon(x)$ is simply

$$\tilde{\varepsilon}(x) = S(x)\varepsilon(x)S^+(x).$$

The new and old gauge potentials $\tilde{A}(x)$ and $A(x)$, however, are related by the more complicated transformation law

$$\tilde{A}(x) = S(x)A(x)S^+(x) - \frac{dS(x)}{dx}S^+(x),$$

well-known from non-abelian gauge theories [8]. The transformed Schrödinger-equation for the longitudinal coefficients then has the same form as (7), i.e.

$$\left[\frac{1}{2M} \left(\hat{p} - i\hbar\tilde{A}(x)\right)^2 + \tilde{\varepsilon}(x)\right]\tilde{\chi}(x) = E\tilde{\chi}(x).$$

Since $\psi(x,y)$ is unchanged, all observables are invariant under this gauge transformation. Choosing a gauge in this context means to choose a certain basis of transverse wave functions at every space point $x$.

The formalism above can now be used to describe the mixing between the different transverse modes – which is formally described by the gauge potential $A(x)$ – in a very explicit form, that also turns out to be convenient for a numerical treatment. To this end a gauge transformation is performed to a gauge in which $\tilde{A}(x) = 0$ vanishes identically. From (11) this requires that

$$\frac{dS(x)}{dx}S(x) = -A(x).$$

This differential equation for the transformation matrix $S(x)$ can be solved formally by

$$S(x,x_0) = R \left[ \exp \int_{x_0}^{x} d\xi A(\xi) \right],$$

where $R$ is the space-ordering operator, defined in complete analogy to the time-ordering operator known from time-dependent perturbation theory. The antisymmetry of the gauge potential $A$ ensures the unitarity of the evolution operator $S(x,x_0)$. In order to understand the physics behind our special gauge, we note that $A$ is defined by

$$\frac{\partial}{\partial x} |n(x)\rangle = -\sum_m A_{nm}(x) |m(x)\rangle.$$

The transverse basis in the gauge where $\tilde{A}(x) = 0$ is therefore obviously the one with a fixed reference point $x_0$. Thus by expanding the total wavefunction in terms of transverse modes which are independent of the longitudinal coordinate $x$, the gauge potential clearly vanishes. The fixed basis set $\Phi_n^x(y)$ is related to the locally adiabatic basis $\Phi_n^x(y)$ at any point $x$ by the unitary transformation $S(x,x_0)$ as given in (14). As a result, the original diagonal matrix $\varepsilon(x)$
of the adiabatic subband energies is transformed to a non-diagonal form via the transformation law (10). Mode-mixing is thus no longer described by a non-vanishing gauge potential but is instead due to the off-diagonal terms in the transformed energy matrix $\tilde{\varepsilon}(x)$.

For an application of the general theory above, it is necessary to specify the confining potential. In order to obtain analytical results as far as possible, we choose a harmonic confinement of the form

$$V(x,y) = M \frac{\omega_0^2}{2} \left( \frac{b_0}{b(x)} \right)^2 y^2.$$  \hspace{1cm} (16)

The effective width $b(x)$ has a minimum $b_0 = b(x = 0)$ at the origin and widens to a finite value $b_\infty = b(x \to \pm \infty)$ at $|x|$ larger than a characteristic constriction length $L$. Quite generally, for a harmonic confining potential, the gauge potential $A(x)$ may be written in the form

$$A(x) = \frac{1}{4} \frac{b'(x)}{b(x)} \left( \hat{a}^2 - \hat{a}^* \right)^2$$ \hspace{1cm} (17)

where $\hat{a}$ is the usual harmonic oscillator destruction operator and the prime denotes differentiation with respect to $x$. Since $A(x)$ factorizes into a simple function of $x$ and a fixed operator, the spatial ordering symbol in (14) is irrelevant in the present case. The evolution operator $S$ is therefore obtained in explicit form as

$$S(x,x_0) = \exp \left[ \frac{1}{4} \ln \left( \frac{b(x)}{b(x_0)} \right) \left( \hat{a}^2 - \hat{a}^* \right) \right].$$  \hspace{1cm} (18)

This operator turns out to be identical with the so called squeeze-operator well known in quantum optics [9]. Its matrix elements in the transverse oscillator eigenstates can be expressed analytically [10] in terms of hypergeometric functions, which are not given here explicitly, however.

In order to solve the coupled differential equations for the longitudinal wave functions $\vec{\chi}(x)$, we eliminate the gauge potential and discretize the transformed equation in steps of size $a$, such that $\vec{\chi}(x = ina) = \vec{\chi}_i$. Transforming back to the original adiabatic basis with a diagonal matrix $\varepsilon(x)$ of subband energies, the resulting equations are

$$\left( \varepsilon_{ii} + 2 \right) \vec{\chi}_i - S_{i+1,i} \vec{\chi}_{i+1} - S_{i-1,i} \vec{\chi}_{i-1} = E \vec{\chi}_i,$$ \hspace{1cm} (19)

in an obvious notation for $\varepsilon_{ii}, S_{i+1,i}$ and with dimensionless energies in units of $\hbar^2/(2Ma^2)$. This is a tight-binding like model in one dimension with as many orbitals per site $i$ as number of transverse modes included (about 20 in the numerical calculations). A convenient and numerically stable method to solve it is the recursive Greenfunction technique [4]. This allows one to calculate the matrix of the local Greenfunctions $G_{mn}(i,j)$ at a given energy $\varepsilon_F$ from which the local density of states

$$\rho(x,y; \varepsilon_F) = -\frac{1}{\pi} \sum_{mn} \Phi^*_m(y) \Phi_n(y) \cdot \text{Im} \ G_{mn}(x,x)$$ \hspace{1cm} (20)

is finally obtained. This quantity can be directly measured in an experiment with a scanning tunneling microscope (STM), provided the two-dimensional electron gas can be realized on a free surface like in InAs-systems. Indeed the local tunneling current between an STM tip and a conducting sample is directly proportional to $\rho(x; \varepsilon_F)$ [11]. In the standard case where the electron gas resides below a surface layer, the LDOS may be determined via a local capacitance spectroscopy as was recently demonstrated by Ashoori [12]. An example for the local density
S. Ulreich and W. Zwerger: Gauge Fields in a Quantum Point Contact

Fig. 1. Local density of states for a quantum point contact with a harmonic confinement of width \( b(x) \) as indicated. In the vicinity of the constriction the “exact” calculation (left) differs strongly from the result obtained in an adiabatic approximation (right).

The local density of states is shown in fig. 1 for a smooth boundary function \( b(x) \) with a width ratio \( b_0/b_\infty = 0.1 \) as indicated in the figure. The characteristic length \( L = 250 \text{ nm} \) while the Fermi energy \( \varepsilon_F = \hbar \omega_0/2 \) is chosen such that it coincides with the lowest transverse mode at the narrowest point \( x = 0 \). Including the quantum mechanical tunneling and reflection over the barrier [5], the associated linear conductance is equal to \( e^2/\hbar \), i.e. we are at the inflection point of the transition between pinch off and the first conductance plateau at \( G = 2e^2/\hbar \). This situation is nicely reflected in the exact calculation of the LDOS shown in fig. 1 on the left, where a narrow dip at the constriction is just about to be closed. In the wide regime where four transverse modes are occupied, the LDOS exhibits a complex interference pattern reflecting the square of the exact wavefunction \( \sum_n \chi_n(x) \Phi_n^x(y) \Phi_n^y(x) \) at the Fermi energy. In this asymptotic regime the structure is reproduced rather well in an adiabatic approximation where all matrices \( S \) in (19) are replaced by a unit matrix. The resulting LDOS is shown in fig. 1 on the right for the same parameter values. It is very similar to the exact result in the regime where \( b(x) \) is constant.

Near the constriction, however, the adiabatic approximation obviously differs strongly from the exact result and in particular it fails to reproduce the almost pinch-off structure. Mode mixing therefore plays a crucial role for local properties like the LDOS.

In conclusion we have developed a novel method to treat quantum scattering in general wave guides via a gauge field approach and have applied it for a calculation of the LDOS in a quantum point contact. The nontrivial local structure found here may possibly be observed using modern scanning probe techniques. Our method can also be used to determine the local potential distribution in the presence of a finite current [13] and the local emissivities and injectivities which determine the ac-transport properties at low frequencies [14].

***

It is a pleasure to acknowledge useful discussions with Bert Lorenz and David Wharam about the possibilities of measuring the LDOS in a quantum point contact. This work was supported by the SFB 348 Nanometer-Halbleiter-Bauelemente.
REFERENCES

[1] van Wees B. J., van Houten H., Beenakker C. W. J., Williamson J. G., Kouwenhouwen L. P., van der Marel D., and Foxon C. T., Phys. Rev. Lett., 60 (1988) 848.

[2] Wharam D. A., Thornton T. J., Newbury R., Pepper M., Ahmed H., Frost J. E. F., Hasko D. G., Peacock D. C., Ritchie D. A., and Jones G. A. C., J. Phys. C, 21 (1988) L209.

[3] Beenakker C. W. J. and van Houten H., in Solid State Physics, edited by H. Ehrenreich and D. Turnbull, Vol. 44 (Academic Press, London) 1991 pp. 1-228.

[4] Maas F., Zozulenko I.V., and Hauge E. H., Phys. Rev. B, 50 (1994) 17320.

[5] Glazman L. I., Lesovik G. B., Khmel’nitskii D. E., and Shekter R. I., JETP Lett., 48 (1988) 238.

[6] Yacoby A. and Imry Y., Phys. Rev. B, 41 (1990) 5341.

[7] Kuperin Yu. A., Kurasov P. B., Melnikov Yu. B., and Merkuriev S. P., Ann. Phys., 205 (1991) 330.

[8] Itzykson C. and Zuber J.-B., Quantum Field Theory, (McGraw-Hill, N.Y.) 1985.

[9] Loudon R. and Knight P. L., Journal of Modern Optics, 34 (1987) 709.

[10] Ulreich S., Thesis LMU (1997) (unpublished).

[11] Tersoff J. and Hamann D. R., Phys. Rev. B, 31 (1985) 805.

[12] Ashoori R. C., Bull. of the APS, 42(1) (1997) 56

[13] Ulreich S. and Zwerger W., Superlattices and Microstructures, submitted (1997).

[14] Büttiker M., J. Phys. Condens. Matt., 5 (1993) 9361