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An abstract approach to the Landauer-Büttiker formula with application to an LED toy model

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joint work with Hagen Neidhardt

Motivation and ideas

Motivation

- Create a simple mathematical (toy) model of a quantum dot LED
- Calculate the electron current through the dot

Model ideas

- Electron-photon interaction via minimal coupling
- Electrons on a lattice
- Localized electron-photon interaction
- Restriction to a single photon

$\rightarrow$ interaction operator is trace class

Currenct calculation

- Independent electrons
- Every electron with individual photon field

$\rightarrow$ Landauer-Büttiker-type formula

The Landauer-Büttiker formula expresses the steady current through a quantum device in terms of the scattering data

$$\mathfrak{J}_j = 2\pi q \int_{\mathbb{R}} d\lambda \sum_{k=1}^{N} \mathrm{Tr}\Big(\widehat{\rho}_j(\lambda)\widehat{T}^*_{jk}(\lambda)\widehat{T}_{jk}(\lambda)\Big) - \mathrm{Tr}\Big(\widehat{\rho}_k(\lambda)\widehat{T}^*_{kj}(\lambda)\widehat{T}_{kj}(\lambda)\Big)$$

Among other approaches, Nenciu [2] derived it from $\rho(t) = e^{itH}\rho\, e^{-itH}$, $[\rho, H_0] = 0$

$$\mathfrak{J}_j = iq\mathrm{Tr}\Big(W_-(H,H_0)\rho W_-^*(H,H_0)[H,P_j]\Big)$$

for trace class perturbations $V = H - H_0$ using

- generalized eigenfunctions ψ_j of H_0 and $\psi_j^\pm = W_\pm(H,H_0)\psi_j$ of H
- Lippmann-Schwinger equation $\psi_j^\pm = \psi_j - (H_0 - \lambda \pm i0)^{-1} V \psi_j^\pm$
- $\widehat{T}_{kj}(\lambda) = \langle \psi_k(\lambda), V W_-(H,H_0)\psi_j(\lambda)\rangle$
- principal value formula $\frac{1}{x-i0} = i\pi\delta(0) + \mathrm{PV}\frac{1}{x}$

In this talk we present a new abstract approach that

- does not use generalized eigenfunctions
- does not use the Lippmann-Schwinger equation
- applies to perturbations V that are only locally trace class

The ideas of the approach are to

- construct a special spectral representation of H_0 using the trace class property of V
- use only the resolvent identity instead of the Lippmann-Schwinger equation
- make use of the relation between T and $VW_-(H, H_0)$ (like Nenciu in [2])
- work with stationary pre-wave operators $W_-(\epsilon)$
- pass to the limit $\epsilon \to +0$ only as a final step

Spectral representation

H_0 selfadjoint operator on $\mathfrak{H}$, spectral measure $E_0(\cdot)$, and $H = H_0 + V$, where $VE_0(\Delta)$ is trace class for some $\Delta \subset \mathbb{R}$.

Now $C_\Delta := \sqrt{|V|}E_0(\Delta)$ is a Hilbert-Schmidt operator and

$$K_\Delta(\lambda) := \frac{dC_\Delta E_0^{ac}((-\infty,\lambda))C_\Delta^*}{d\lambda} \geq 0$$

is trace class. If $\mathfrak{H}^{ac} := E_0^{ac}(\Delta)\mathfrak{H} = \overline{\mathrm{span}\{E_0^{ac}(\delta)\mathrm{ran}(C_\Delta)|\delta \in \mathcal{B}(\Delta)\}}$, then

$$\big(\Phi_\Delta E_0^{ac}(\delta)C_\Delta f\big)(\lambda) := \chi_\delta(\lambda)\sqrt{K_\Delta(\lambda)}f, \quad f \in \mathfrak{H}$$

extends to isometric isomorphism $\Phi_\Delta : \mathfrak{H}^{ac} \to L^2(\Delta, d\lambda, \mathfrak{H}_\lambda), \mathfrak{H}_\lambda = \overline{\mathrm{ran}\big(K_\Delta(\lambda)\big)}$.

We have the relations

$$\left(\Phi_\Delta \int_\Delta dE_0^{ac}(\mu)C_\Delta^* A(\mu)f\right)(\lambda) = \sqrt{K_\Delta(\lambda)}A(\lambda)f$$

$$\int B(\mu)C_\Delta dE_0^{ac}(\mu)\Phi_\Delta^* \widehat{f} = \int d\mu B(\mu)\sqrt{K_\Delta(\mu)}\widehat{f}(\mu)$$

Consider the stationary pre-wave operators

$$W_\pm(\epsilon) = P_0^{ac} - \widetilde{W}_\pm(\epsilon)\int_{\mathbb{R}} \big(1 - (H - \lambda \pm i\epsilon)^{-1}V\big)dE_0^{ac}.$$

We have

$$\big(\Phi_\Delta E_0^{ac}(\Delta)VW_-(H,H_0)\Phi_\Delta^*\widehat{f}\big)(\lambda)$$

$$= s - \lim_{\epsilon\to+0}\Bigg(\Phi_\Delta \iint_{\Delta\times\Delta} dE_0^{ac}(\nu)C_\Delta^*(J - JC(H_A - \mu - i\epsilon)^{-1}CJ)C_\Delta dE_0^{ac}(\mu)\Phi_\Delta^*\widehat{f}\Bigg)(\lambda)$$

$$= s - \lim_{\epsilon\to+0}\sqrt{K_\Delta(\lambda)}\int_\Delta d\mu M(\mu + i\epsilon)\sqrt{K_\Delta(\mu)}\widehat{f}(\mu)$$

for $\widehat{f} \in L^2(\Delta, d\lambda, \mathfrak{H}_\lambda)$. We know from abstract theory (cf. [3]) that

$$\widehat{T}(\lambda) = \big(\Phi_\Delta E_0^{ac}(\Delta)VW_-(H,H_0)\Phi_\Delta^*\big)(\lambda,\lambda).$$

Hence,

$$\widehat{T}(\lambda) = s - \lim_{\epsilon\to+0}\sqrt{K_\Delta(\lambda)}M(\lambda + i\epsilon)\sqrt{K_\Delta(\lambda)},$$

or in terms of the scattering matrix

$$\widehat{S}(\lambda) = I_{\mathfrak{H}_\lambda} - 2\pi i\sqrt{K_\Delta(\lambda)}M(\lambda + i0)\sqrt{K_\Delta(\lambda)}.$$

$$
\begin{aligned}
&\lim_{\epsilon\to+0} \frac{1}{2i}\mathrm{Tr}\Big(W_-(\epsilon)\rho E_0^{ac}(\Delta)W_-^*(\epsilon)[V,P_j]\Big)\\
&= \lim_{\epsilon\to+0} \Im\mathrm{m}\Big[\mathrm{Tr}\Big(\Phi_\Delta \rho E_0^{ac}(\Delta)W_-^*(\epsilon)VP_jW_-(\epsilon)E_0^{ac}(\Delta)\Phi_\Delta^*\Big)\Big]\\
&= \lim_{\epsilon\to+0}\int_\Delta d\lambda \Im\mathrm{m}\Big[\mathrm{Tr}\Big(\widehat{\rho}(\lambda)\sqrt{K_\Delta(\lambda)}M(\lambda-i\epsilon)\sqrt{K_\Delta(\lambda)}\widehat{P}_j(\lambda)\Big)\Big]\\
&\quad - \lim_{\epsilon\to+0} \Im\mathrm{m}\Big[\mathrm{Tr}\Big(\Phi_\Delta \rho E_0^{ac}(\Delta)W_-^*(\epsilon)VP_j\\
&\qquad \times \int_\Delta \underbrace{(H_0-\nu-i\epsilon)^{-1}(1-V(H-\nu-i\epsilon)^{-1})}_{=(H-\nu-i\epsilon)^{-1}} V dE_0^{ac}(\nu)\Phi_\Delta^*\Big)\Big]\\
&= \int_\Delta d\lambda \Im\mathrm{m}\Big[\widehat{\rho}(\lambda)\widehat{T}^*(\lambda)\widehat{P}_j(\lambda)\Big]\\
&\quad - \lim_{\epsilon\to+0}\int_\Delta d\lambda \mathrm{Tr}\Big(\widehat{\rho}(\lambda)\sqrt{K_\Delta(\lambda)}M(\lambda-i\epsilon)\int_\Delta d\mu\sqrt{K_\Delta(\mu)}\widehat{P}_j(\mu)\\
&\qquad \times \sqrt{K_\Delta(\mu)}\frac{\epsilon}{(\mu-\lambda)^2+\epsilon^2}M(\lambda+i\epsilon)\sqrt{K_\Delta(\lambda)}\Big)
\end{aligned}
$$

Now the limit $\epsilon \to +0$ and the optical theorem $\Im\mathrm{m}[\widehat{T}^*(\lambda)] = -\pi\widehat{T}^*(\lambda)\widehat{T}(\lambda)$ gives us

$$\begin{aligned}
&\lim_{\epsilon\to+0} \mathrm{Tr}\Big(W_-(\epsilon)\rho E_0^{ac}(\Delta)W_-^*(\epsilon)[V, P_j]\Big) \\
&\quad = \pi \int_\Delta d\lambda \mathrm{Tr}\Big(\widehat{\rho}(\lambda)\widehat{T}^*(\lambda)\widehat{P}_j(\lambda)\widehat{T}(\lambda)\Big) - \mathrm{Tr}\Big(\widehat{\rho}(\lambda)\widehat{T}^*(\lambda)\widehat{T}(\lambda)\widehat{P}_j(\lambda)\Big) \\
&\quad = \pi \int_{\mathbb{R}} d\lambda \sum_{k=1}^{N} \mathrm{Tr}\Big(\widehat{\rho}_k(\lambda)\widehat{T}_{kj}^*(\lambda)\widehat{T}_{kj}\Big) - \mathrm{Tr}\Big(\widehat{\rho}_j(\lambda)\widehat{T}_{jk}^*(\lambda)\widehat{T}_{jk}\Big),
\end{aligned}$$

which corresponds to the Landauer-Büttiker formula in the introduction.

The electron is modelled by

- the Hilbert space $\mathfrak{h}^e = L^2(\mathbb{Z} \times \Lambda) = \mathfrak{h}^e_L \oplus \mathfrak{h}^e_S \oplus \mathfrak{h}^e_R$ with finite dimensional $\mathfrak{h}^e_S$
- a decoupled Hamiltonian $h^e_0 = h^e_L \oplus h^e_S \oplus h^e_R$
- $h^e_x = -\Delta^D + v_x, x \in \{L, S, R\}$, where $v_L = v_R = \mathrm{const}$
- a coupled Hamiltonian $h^e = h^e_0 + v_a$, where the coupling v_a is trace class and h^e_0-smooth
- in our case the coupling v_a is even finite dimensional

Application to an LED toy model - The model (photon)

The photon field is modelled in the following way

- the full Hilbert space is the symmetric Fock space $\mathcal{F}_+(L^2(\mathbb{R}^d))$
- the free Hamiltonian is $d\Gamma(M_\omega) = \int_{\mathbb{R}^3} dk\, \omega(k) a^*(k) a(k),\ \omega(k) = |k|$
- the vector potential is $A_{\mathcal{F}}(x) = a^*(G_x) + a(G_x)$ with

$$G_x(k) = \frac{\kappa(|k|)}{\sqrt{|k|}} \epsilon(k) e^{i\alpha x k}$$

- we take the zero or one photon subspace $\mathbb{C} \oplus L^2(\mathbb{R}^d)$ of $\mathcal{F}_+(L^2(\mathbb{R}^d))$
- the free Hamiltonian is then $h^p = \begin{pmatrix} 0 & 0 \\ 0 & M(\omega) \end{pmatrix}$
- additionally, restriction of the vector potential to a bounded region $\Xi \times \Lambda \subset \mathbb{Z} \times \Lambda$
- the vector potential becomes

$$A(x) = \begin{pmatrix} 0 & \langle \chi_\Xi(x) G_x | \\ | \chi_\Xi(x) G_x \rangle & 0 \end{pmatrix}$$

The full model

- the Hilbert space $\mathfrak{H} = \mathfrak{h}^e \otimes \mathfrak{h}^p = \mathfrak{h}^e \oplus \mathfrak{h}^e \otimes L^2(\mathbb{R}^d)$
- we use minimal coupling to derive the full Hamiltonian

$$\widetilde{H}_0 = \big(-i\nabla_x^D \otimes I_2 + \alpha^{\frac{3}{2}} A(x) \big)^2 + I_1 \otimes h^p$$

- for simplicity, drop the A^2-term (bounded operator)
- from this we get our electron-field interaction

$$V_B = \begin{pmatrix} 0 & -i\alpha^{\frac{3}{2}} \nabla_x^D \chi_\Xi(x) \langle G_x | \\ -i\alpha^{\frac{3}{2}} \chi_\Xi(x) \nabla_x^D | G_x \rangle & 0 \end{pmatrix}$$

- this is a finite dimensional operator since $\mathfrak{h}_S^e$ is finite dimensional
- the decoupled Hamiltonian $H_0 = h_0^e \otimes 1 + 1 \otimes h^p$
- the electron-coupled Hamiltonian $H_A = H_0 + V_A$, where $V_A = v_A \otimes 1$
- the fully coupled Hamiltonian $H_B = H_A + V_B$

The wave operator

$$W_- \equiv W_-(H_B, H_0) = W_-(H_B, H_A)\big(W_-(h^e, h_0^e) \otimes 1\big) \equiv W_{B,-}W_{A,-}$$

exists only on $P := (P_{ac}(h_0^e) \otimes 1)\mathfrak{H}$. The electron current is formally given by

$$\mathfrak{J}_j = iq\mathrm{Tr}\Big(W_{B,-}W_{A,-}\rho\, W_{A,-}^* W_{B,-}^* \big[V_A + V_B, P_j \otimes 1\big]\Big),$$

where

- the electrons are non-interacting
- every electron has its own photon field

$\rightarrow$ no photon-mediated electron interaction

$\rightarrow$ no emission and reabsorption

The total perturbation $V_A + V_B$ is not trace class, but v_A is.

$\rightsquigarrow$ apply same methods and make use of the tensor structure (work in progress!)

Application to an LED toy model - The ideas

Initial state $[\rho^e, h_0^e] = 0$ and

$$\rho = \begin{pmatrix} \rho^e & 0 \\ 0 & 0 \end{pmatrix} = \rho^e \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

i.e., leads and system in equilibrium, no photons present.

Then obviously $1 - W_{B,-}(\epsilon)$, but also

$$\rho W_{A,-}^*(\epsilon) V_A = \rho^e W_-^*(h^e, h_0^e) v_a \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

is trace class. Thus, the electron current

$$\mathfrak{J}_j = -\lim_{\epsilon \to +0} 2q\Im\mathrm{m}\Big[\mathrm{Tr}\Big(P\rho\, W_{A,-}^*(\epsilon) W_{B,-}^*(\epsilon)\big(V_A + V_B\big) P_j W_{B,-}(\epsilon) W_{A,-}(\epsilon)\Big)\Big],$$

is well defined.

Note that

$$T = T_A + W_{A,+}^* T_B W_{A,-}$$

Now use

$$PW^*_{A,-}(\epsilon)W^*_{B,-}(\epsilon)\big(V_A + V_B\big) \\ = W^*_{A,-}(\epsilon)V_A P + W^*_{A,-}(\epsilon)W^*_{B,-}(\epsilon)V_B W_{A,+}(\epsilon) + F^*(\epsilon)$$

to get the terms of the electronic Landauer-Büttiker formula

$$\mathrm{Tr}\big(\rho W^*_{A,-}(\epsilon)V_A P\big) \rightsquigarrow \int_{\mathbb{R}} d\lambda \mathrm{Tr}\big(\widehat{\rho}(\lambda)\widehat{T}^*_A(\lambda)\widehat{P}(\lambda)\big),$$

$$\Im\mathrm{m}\big[\mathrm{Tr}\big(\rho W^*_{A,-}(\epsilon)V_A P\widetilde{W}^*_{A,-}(\epsilon)\big)\big] \rightsquigarrow \int_{\mathbb{R}} d\lambda \mathrm{Tr}\big(\widehat{\rho}(\lambda)\widehat{T}^*_A(\lambda)\widehat{P}(\lambda)\widehat{T}_A(\lambda)\big),$$

and correction terms due to the interaction like

$$W^*_{A,-}(\epsilon)W^*_{B,-}(\epsilon)V_B W_{A,+}(\epsilon) + F(\epsilon) \rightsquigarrow \widehat{W}^*_{A,-}(\lambda)\widehat{T}_B(\lambda)\widehat{W}_{A,+}(\lambda),$$

and similarly

$$\widehat{W}^*_{A,-}(\lambda)\widehat{T}_B(\lambda)\widehat{W}_{A,+}(\lambda)\widehat{P}(\lambda)\widehat{T}_A(\lambda),$$

$$\widehat{T}_A(\lambda)\widehat{P}(\lambda)\widehat{W}^*_{A,+}(\lambda)\widehat{T}_B(\lambda)\widehat{W}_{A,-}(\lambda)$$

$$\widehat{W}^*_{A,-}(\lambda)\widehat{T}_B(\lambda)\widehat{W}_{A,+}(\lambda)\widehat{P}(\lambda)\widehat{W}^*_{A,+}(\lambda)\widehat{T}_B(\lambda)\widehat{W}_{A,-}(\lambda).$$

References

[1] M. Büttiker, Y. Imry, R. Landauer, and S. Pinhas, *Generalized many-channel conductance formula with application to small rings*, Phys. Rev. B **31** (1985), no. 10, 6207–6215.

[2] G. Nenciu, *Independent electron model for open quantum systems: Landauer-Buttiker formula and strict positivity of the entropy production*, J. Math. Phys. **48** (2007), no. 3, 033302.

[3] Hellmut Baumgärtel and Manfred Wollenberg, *Mathematical Scattering Theory*, Akademie-Verlag, 1983.