



Convexity of trace functionals and Schrödinger operators

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Abstract

Let H be a semi-bounded self-adjoint operator on a separable Hilbert space. For a certain class of positive, continuous, decreasing, and convex functions F we show the convexity of trace functionals of the form $\text{tr}(F(H + U - \varepsilon(U))) - \varepsilon(U)$, where U is a bounded, self-adjoint operator and $\varepsilon(U)$ is a normalizing real function—the Fermi level—which may be identical zero. If additionally F is continuously differentiable, then the corresponding trace functional is Fréchet differentiable and there is an expression of its gradient in terms of the derivative of F . The proof of the differentiability of the trace functional is based upon Birman and Solomyak's theory of double Stieltjes operator integrals. If, in particular, H is a Schrödinger-type operator and U a real-valued function, then the gradient of the trace functional is the quantum mechanical expression of the particle density with respect to an equilibrium distribution function $f = -F'$. Thus, the monotonicity of the particle density in its dependence on the potential U of Schrödinger's operator—which has been understood since the late 1980s—follows as a special case.

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1. Introduction

In the semi-classical approximation the density of electrons and holes in a two-band bulk semiconductor depends continuously and monotone on the chemical potential of electrons and holes, respectively. This behaviour of the charge densities ensures the unique solvability of Poisson's equation for the electrostatic potential, see, e.g., [9,10,26] and the references cited there.

In quantum semiconductor structures like resonant tunneling diodes and quantum well lasers the semi-classical approximation and its underlying assumption, that electrons and holes can move freely in all space directions, is not valid anymore. Instead, in a quantum well a quantization of energy levels takes place, see, e.g., [7,29]. The electron density in quasi low-dimensional systems, such as quantum-wells, -wires, and -dots in the infinitely high barriers limit, is obtained by solving an eigenvalue problem

$$(H + U)\psi_j(U) = \lambda_j(U)\psi_j(U)$$

for an appropriate Hamiltonian $H + U$ with pure point spectrum on a space of square integrable functions. More precisely, the electron density is given by

$$\sum_{j \in \mathbb{N}} f(\lambda_j(U) - \varepsilon(U)) |\psi_j(U)(x)|^2,$$

where f is the thermodynamic equilibrium distribution function for the system and ε is the quasi-Fermi potential which in general also depends on U . The shift $\varepsilon(U)$ normalizes the trace of $f(H + U - \varepsilon(U))$ in such a way that $f(H + U - \varepsilon(U))$ becomes a density matrix. In this paper we normalize to 1, though other conventions are also common. In semiconductor physics— H being a one-electron, effective mass Hamiltonian in Ben–Daniel–Duke form—one often chooses the total number of undistinguishable electrons in the system as normalizing condition. If the thermodynamic equilibrium distribution function f is smooth enough, strictly and sufficiently rapidly decreasing, then the electron density depends—as in the semi-classical approximation—continuously and anti-monotone on the potential of the Hamiltonian, which is, up to the normalizing shift, the negative chemical potential. This fact has been observed in 1990 independently by Caussignac et al. [6] and Nier [23] for the spatially one-dimensional case. In [13–16,24] the monotonicity result for the electron density has been extended to larger classes of thermodynamic equilibrium distribution functions f , to two and three space dimensions (that means to quantum wires and quantum dots) including the case of quantum heterostructures with mixed boundary conditions. As in the semi-classical approximation the monotonicity result for the electron and hole density has been used to prove existence and uniqueness of solutions for the corresponding non-linear Poisson equation, then usually addressed as Schrödinger–Poisson system [6,13–16,23,24]. Even more, one obtains existence and conditional uniqueness of solutions for the Euler equations of density functional theory—in local density approximation—the so called Kohn–Sham system [15,16].

In this paper we generalize the monotonicity result for the density to abstract quantum systems with an unperturbed Hamiltonian H which has pure point spectrum. Making minimal requirements on the continuity and the decay of the thermodynamic equilibrium distribution function f we prove that the density matrix $f(H + U - \varepsilon(U))$ is the negative gradient of the convex functional

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