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J. Phys. A: Math. Theor. 41 (2008) 405203 (4pp)

doi:10.1088/1751-8113/41/40/405203

A proof of the Kramers degeneracy of transmission eigenvalues from antisymmetry of the scattering matrix

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Received 20 May 2008 Published 15 September 2008 Online at stacks.iop.org/JPhysA/41/405203

Abstract

In time-reversal-symmetric systems with half integral spins (or more concretely, systems with an antiunitary symmetry that squares to -1 and commutes with the Hamiltonian) the transmission eigenvalues of the scattering matrix come in pairs. We present a proof of this fact that is valid for both even and odd number of modes and relies solely on the antisymmetry of the scattering matrix imposed by time reversal symmetry.

PACS numbers: 73.23.-b, 05.60.Gg, 03.65.Nk

1. Introduction

In the early days of quantum mechanics, Kramers noticed a highly consequential feature of the Schrödinger equation with spin [1]. In the absence of a magnetic field, he found a transformation *T* such that if $|\psi\rangle$ is an eigenstate with energy *E*, then $T|\psi\rangle$ is also an eigenstate. Furthermore, if the system has a half-integral spin, these two eigenstates are orthogonal and the spectrum is twofold degenerate. This degeneracy is the celebrated *Kramers degeneracy* (of energy eigenvalues).

A couple of years after Kramers' discovery, Wigner pointed out that the transformation T is simply time reversal and that the degeneracy is a manifestation of time reversal symmetry [2]. In general, Wigner has shown that all symmetry operations can be represented by either an unitary (and linear) or an antiunitary (and antilinear) operator that commutes with the Hamiltonian [3]. In the case of time reversal, the operator T is antiunitary. Furthermore, the square of the time-reversal operator equals plus or minus one [3]. For half-integral spin $T^2 = -1$ while for integral spin $T^2 = 1$. Thus, the mathematical conditions for Kramers degeneracy are that there exists an antiunitary operator T with $T^2 = -1$, which commutes with the Hamiltonian $H(T^2 = -1)$ is needed to guarantee that $|\psi\rangle$ and $T|\psi\rangle$ are orthogonal). Time reversal symmetry is just one example of a symmetry that is represented by an antiunitary operator, but since all antiunitary operators can be written as a product of an unitary operator and the time-reversal operator one generally just speaks of time reversal.

1751-8113/08/405203+04\$30.00 © 2008 IOP Publishing Ltd Printed in the UK

A more recently appreciated consequence of time reversal symmetry is the fact that in two-terminal scattering of systems with half-integral spin, the transmission eigenvalues (eigenvalues of the transmission matrix product tt^{\dagger}) also come in Kramers degenerate pairs. This is a less intuitive result than for the energy eigenvalues. In fact, one expects an electron moving in some direction to have the same energy as an electron moving in the opposite direction. In terms of scattering, however, time reversal connects incoming states to outgoing states, making it less obvious that there should be any degeneracy in the transmission eigenvalues.

In this paper we give a new proof of this Kramers degeneracy of the transmission eigenvalues. There are at least two reasons why this might be beneficial. Firstly, the proofs of this statement that exist in the literature [4, 5] are not given directly in terms of the scattering matrix through which the transmission eigenvalues are obtained, but rather by use of the transfer matrix. While this is equivalent, it tends to obscure and make the proofs by far less accessible than the proof of the corresponding theorem for energy levels [6]. Secondly, these proofs rest on the quaternionic structure of the transfer and scattering matrices and are thus strictly only applicable to systems with an even number of modes, while Kramers degeneracy is also present for systems with an odd number of modes.

2. The proof

The proof consists of two steps. In the first step we introduce a basis in which the scattering matrix is found to be antisymmetric. In the second step we use the resulting antisymmetry of the matrix of reflection amplitudes to show that the transmission eigenvalues necessarily come in pairs.

Consider thus a two-terminal scattering setup with N_L (N_R) propagating modes in the left (right) lead. Assume further that the system has a time reversal (antiunitary) symmetry T that squares to minus one, $T^2 = -1$. We denote the incoming modes on the left (right) with $|n\rangle$ ($|m\rangle$). The outgoing modes on the left (right) are then $T|n\rangle = |Tn\rangle$ ($T|m\rangle = |Tm\rangle$). Since $\langle n|Tn\rangle = 0$ as a consequence of the properties of T, it is straightforward to show (for example using the Gram–Schmidt procedure) that the basis { $|n\rangle$, $|Tn\rangle$ } can always be chosen to be orthogonal. A general scattering state $|\psi\rangle$ will thus have the form

$$|\psi\rangle = \sum_{n=1}^{N_L} \left(c_n^{\text{in,L}} |n\rangle + c_n^{\text{out,L}} |Tn\rangle \right) \tag{1}$$

in the left lead, and similar in the right lead (with $n \to m$ and $L \to R$). The vectors of coefficients c^{in} and c^{out} are related by the scattering matrix S,

$$\begin{pmatrix} c^{\text{out},\mathsf{L}} \\ c^{\text{out},\mathsf{R}} \end{pmatrix} = S \begin{pmatrix} c^{\text{in},\mathsf{L}} \\ c^{\text{in},\mathsf{R}} \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} c^{\text{in},\mathsf{L}} \\ c^{\text{in},\mathsf{R}} \end{pmatrix}.$$
(2)

Due to time reversal symmetry,

$$T|\psi\rangle = \sum_{n=1}^{N_L} \left[\left(c_n^{\text{in},\text{L}} \right)^* |Tn\rangle - \left(c_n^{\text{out},\text{L}} \right)^* |n\rangle \right]$$
(3)

is also a scattering state with the same energy. This means that

$$\begin{pmatrix} (c^{\mathrm{in},\mathrm{L}})^*\\ (c^{\mathrm{in},\mathrm{R}})^* \end{pmatrix} = S \begin{pmatrix} -(c^{\mathrm{out},\mathrm{L}})^*\\ -(c^{\mathrm{out},\mathrm{R}})^* \end{pmatrix}.$$
(4)

Using unitarity of S we conclude, by comparison with equation (2), that in our chosen basis S is antisymmetric

$$S^T = -S. (5)$$

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We note that if the outgoing states come in pairs, such that if $T|n\rangle$ is an outgoing state $i\sigma_2 T|n\rangle$ is also an outgoing state, it is most common to pair $|n\rangle$ and $i\sigma_2 T|n\rangle$ rather than $|n\rangle$ and $T|n\rangle$ as we have done (this way the pairs have the same spin, while in our case it is opposite). In this case the scattering matrix is found to be self-dual [7] $\sigma_2 S^T \sigma_2 = S$. It is, however, not always possible to find such pairing (one example where it is possible is the usual case of metallic leads with electrons of spin half and no spin–orbit coupling), and we will therefore use the more general representation (1) in which S is antisymmetric.

As a consequence of the antisymmetry of the scattering matrix, the $N_L \times N_L$ matrix of reflection amplitudes *r* is also antisymmetric. Being antisymmetric *r* can be decomposed [8, 9] as $r = W^T DW$, with *W* a unitary matrix and

$$D = \Sigma_1 \oplus \Sigma_2 \oplus \dots \oplus \Sigma_k \oplus 0 \oplus \dots \oplus 0, \tag{6}$$

where $2k = \operatorname{rank} r$, \oplus denotes the direct sum and

$$\Sigma_j = \begin{pmatrix} 0 & \lambda_j \\ -\lambda_j & 0 \end{pmatrix}, \qquad \lambda_j > 0, \qquad j = 1, \dots, k.$$
(7)

In other words, D is block diagonal with $k \ 2 \times 2$ nonzero blocks Σ_j and $N_L - 2k \ 1 \times 1$ zero blocks 0. Clearly, if there are an odd number of modes (i.e. the dimension of r is odd) there is at least one zero block in the sum (6). Using this result, we find that

$$r^{\dagger}r = W^{\dagger}D^{T}DW.$$
(8)

But since

$$\Sigma_j^T \Sigma_j = \begin{pmatrix} \lambda_j^2 & 0\\ 0 & \lambda_j^2 \end{pmatrix},\tag{9}$$

the matrix $D^T D$ is diagonal. We have thus managed to diagonalize $r^{\dagger}r$ and found that its eigenvalues come in pairs. Due to unitarity of S, $1 - r^{\dagger}r$ and $t^{\dagger}t$ have the same eigenvalues. The transmission eigenvalues are thus twofold degenerate, plus (if the number of modes is odd) one transmission eigenvalue equal to unity (perfect transmission [10]). This is the Kramers degeneracy of transmission eigenvalues.

3. Conclusion

In conclusion, we have presented, using only the symmetry of the scattering matrix, a concise proof of the fundamental fact that in the presence of time reversal symmetry and for half-integral spin the transmission eigenvalues of the two terminal scattering matrix come in (Kramers) degenerate pairs.

Acknowledgment

I thank C W J Beenakker for helpful discussions.

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