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Eigenvalue asymptotics related to impurities in crystals.

Rainer Hempel

1. Introduction.

In the present paper, we continue the analysis of eigenvalues of Schrödinger operators $H - \lambda W$ in a spectral gap of H. As a typical example, one should think of $H = -\Delta + V$ as a periodic Schrödinger operator which, in solid state physics, may be used to describe the energy spectrum of an electron moving in a pure crystal (in the so-called 1-electron model). The perturbation W simulates a localized impurity, and $\lambda \in \mathbf{R}$ is a coupling constant; both V and W are assumed to be real-valued. Here we ask for the existence and number of discrete eigenvalues of $H - \lambda W$ which are moved into or through the gap as λ increases from 0 to ∞ . The connection of this question to solid state physics is discussed in more detail in [7,13]; we only mention that "impurity levels" (i. e., energy levels which are introduced into the spectral gap of the pure crystal by impurities) are responsible for the color of crystals in the case of insulators, and strongly influence conductivity in the case of semi-conductors; cf., e. g., [3, 21].

In the mathematical analysis of this problem, it turns out that the case where W doesn't change sign enjoys many simplifying features: fixing E in the gap and assuming $W \ge 0$ for the moment, basic existence and asymptotic results can be read off from the associated (compact and symmetric) Birman-Schwinger kernel $W^{1/2}(H-E)^{-1}W^{1/2}$, (cf. Klaus [18] and, most recently, the remarkable work of Birman [4]). This approach is based entirely on functional analysis and avoids PDE-methods.

In the general situation where W changes sign, however, the associated Birman-Schwinger kernel is no longer symmetric and it is hard to extract useful information from its analysis. Here a more direct approach was developed by Deift and Hempel [7] which combines localization techniques and a quasi-classical volume counting in phase space. Led by some simple physical intuition—which says that a localized perturbation should have localized effects— we start from a suitable approximating problem on the ball B_n , and let n tend to ∞ . Note, however, that even this approximation step is by no means trivial, since restricting the operator $-\Delta + V$ to B_n and imposing Dirichlet boundary conditions, will in general produce (unwanted!) eigenvalues in the gap. This method was further extended in some work of Hempel [13, 15], Alama, Deift and Hempel [1], where decoupling by an additional Dirichlet boundary

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condition (DBC) or Neumann boundary condition (NBC) on ∂B_R is used to separate the region where the perturbation λW is active from the remaining portion of B_n . In Section 2, below, a brief outline of this technique is given (for a more detailed description, cf. [1,15]). By now, this approach has been fully developed and it provides various asymptotic results for the eigenvalue counting functions N_{\pm} , where

$$N_{\pm}(\lambda; H - E, W) = \sum_{0 < \mu < \lambda} \dim \ker(H \mp \mu W - E)$$
(1.1)

counts the number of crossings of eigenvalue branches, keeping track of multiplicities; here, again, E is a fixed "control point" in the gap. In Section 3, we present upper and lower asymptotic bounds on N_+ in the general case $W = W_+ - W_-, W_{\pm} \ge 0.$

In Section 4, finally, our method will be used in the delicate problem of finding a lower bound for the (finite) quantity

$$N_{-}(\infty; K) := \sup_{\lambda > 0} N_{-}(\lambda; H - E, \chi_K),$$

where K is a fixed compact subset of \mathbb{R}^{ν} . $N_{-}(\infty; K)$ counts the total number of eigenvalue branches which cross E under the influence of a potential "barrier" supported on K, with height going to infinity. While it is known that (in dimension > 2) no eigenvalue branch of $H + \lambda \chi_K$, $\lambda > 0$, will ever cross E if the diameter of K is small enough, we also know that some eigenvalues will cross E if K contains a ball of sufficiently large radius (cf.[13,15]). In the present paper, we'll concentrate on K's which are drastically different from balls. Here it turns out that decoupling by natural DBC plays a crucial role, highlighting once more the fundamental difference between N_+ and N_- in the case where W is non-negative: while N_+ is dominated by the Weyl term, which is related to the volume of the interior of K, the number we are investigating now is more or less independent of the volume of K; e. g., a set K looking like a swiss cheese with many small holes may be very effective in shifting eigenvalues through the gap although the volume of the cheese might be very small as compared with the volume of the holes.

The approach described above allows us to discover some of the local effects of the perturbation and connects phase space analysis with eigenvalue counting. However, it is neither simple nor short, and there are many results which can be obtained by more direct methods; we conclude this introduction with a brief discussion of some of these alternatives. As mentioned above, a very fruitful idea consists in the recent observation of Birman [4] that one should apply the first resolvent equation to $(H - E)^{-1}$ in the Birman-Schwinger kernel to replace the control point E in the gap by some $E_0 < \inf \sigma(H)$. The transformed kernel can then be analyzed with the aid of the Gokhberg-Krein theory of weak trace ideals. This yields some sharp asymptotic results for N_+ in the case where Wis non-negative, and works even for E sitting on the gap edge, if H is periodic. Since this method tests asymptotics on the scale of Weyl's Law, it gives only weak information for N_- , however.

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For W changing sign, W of compact support, a very short and elegant proof for the existence of eigenvalues of $H - \lambda W$ in the gap has been given by Gesztesy and Simon [11], while some very detailed and surprising facts concerning the trajectories of eigenvalue branches in the o.d.e.-case ("trapping and cascading") have been discovered by Gesztesy et al. [10]. Of particular interest and difficulty is the question for the number of eigenvalues in a given *interval* in the gap; here we would like to mention some recent 1-dimensional work of Sobolev [28]. For results concerning eigenvalues in gaps under the semi-classical point of view, we refer to Klopp [19] and Outassourt [20]. Finally, Alama and Li [2] have created a non-linear Birman-Schwinger principle which can be successfully applied to non-linear perturbations of periodic Schrödinger operators.

2. Approximation and decoupling.

We are now going to give a condensed description of the approach developed by Deift and Hempel; for details, see [1,15]. Starting from a Schrödinger operator $H = -\Delta + V$, where V is a bounded potential and H is the unique self-adjoint extension of $-\Delta + V$ on $C_c^{\infty}(\mathbf{R}^{\nu})$, we make the *basic assumption* that $\sigma(H)$, the spectrum of H, has a gap. Again, we are mainly interested in the case where the spectral gap occurs above the infimum of $\sigma_{ess}(H)$, the essential spectrum of H. As a typical example, one may think of H as a periodic Schrödinger operator, but spectral gaps may also occur in Schrödinger operators of disordered matter (Briet, Combes and Duclos [5]). Also, for convenience, we assume that $V \geq 1$. In the sequel, let a < b be such that

$$[a,b] \cap \sigma(H) = \emptyset.$$

We next introduce the perturbation W, a bounded, real-valued function going to 0 at infinity. While $H - \lambda W$ has the same essential spectrum as H, the perturbation λW may produce discrete spectrum in the gap. By Kato-Rellich perturbation theory, the eigenvalues of $H - \lambda W$ depend analytically on the coupling constant λ , as long as they stay inside the gap. In order to count the eigenvalues, we now fix $E \in (a, b)$ and we define $N_{\pm}(\lambda) := N_{\pm}(\lambda; H - E, W)$ as in (1.1).

In the case of non-negative W there are some nice quasi-classical heuristics ("volume counting in phase space"; cf. [7,1]) which suggest that one should expect for N_+ an asymptotic behavior with a leading order term as in Weyl's Law,

$$N_+(\lambda) \sim c_{\nu} \lambda^{\nu/2} \int W^{\nu/2}, \quad \lambda \to \infty,$$

if W decays faster than quadratically. In contrast, if W behaves like $c|x|^{-\alpha}$, for x large and some constants $c, \alpha > 0$, then N_{-} is highly dependent on the decay rate α ,

$$N_{-}(\lambda) \sim C \cdot \lambda^{\nu/\alpha}, \quad \lambda \to \infty,$$

under certain natural assumptions on W (cf. [1]). Note that the asymptotics of N_+ can be obtained by Birman's method in [4], and this even in the case

where E is situated on the edge of a gap. The case where W changes sign is much harder to understand, and there are only a few upper and lower bounds on $N_{+}(\lambda)$, for λ large; this will be discussed in Section 3 in more detail.

We next describe the sequence of approximating problems which are used to compactify the problem. Let a' < a and b' > b be such that the interval [a', b'] doesn't intersect the spectrum of H. As in [13,1,15], we define

$$H_n = -\Delta_n + V|_{B_n},$$

where $-\Delta_n$ denotes the Dirichlet Laplacian on the ball B_n in \mathbf{R}^{ν} , and we consider the spectral projection $\Pi_n = P_{[a',b']}(H_n)$ associated with the interval [a',b'] where $\{P_{\lambda}\}_{\lambda \in \mathbf{R}}$ denotes the spectral family. Clearly, Π_n is finite dimensional, and for c' = b' - a', we have

$$\sigma \left(H_n + c' \Pi_n \right) \cap \left(a', b' \right) = \emptyset.$$

In the next step, we apply cut-offs in order to restrict the integral operator Π_n to the region $B_n - B_{n/2}$. Letting ψ_n be defined by $\psi_n(x) = \psi(x/n), x \in \mathbf{R}^{\nu}$, $n \in \mathbf{N}$, where $\psi \in C^{\infty}(\mathbf{R}^{\nu})$ enjoys the properties $\psi(x) = 1$, for $|x| \geq 3/4$, $\psi(x) = 0$, for $|x| \leq 1/2$, and $0 \leq \psi(x) \leq 1$ else, we define

$$\ddot{H}_n = H_n + c' \psi_n \Pi_n \psi_n.$$

Here the important point is that H_n has a spectral gap containing the interval [a, b], for sufficiently large n, i. e.,

$$\sigma(H_n) \cap [a,b] = \emptyset, \quad n \ge n_0.$$

This basic result is a consequence of Weyl's Law (which yields a bound dim $\Pi_n \leq cn^{\nu}$) and the fact that the eigenfunctions of H_n which build up the projection Π_n are exponentially localized near the boundary ∂B_n (cf. [7,1] for details).

The second useful fact is that the Birman-Schwinger kernels associated with \tilde{H}_n and $W|_{B_n}$ converge to the full Birman-Schwinger kernel in norm. This in turn implies the following comparison result for the counting functions ([15; Proposition 2.3]), valid for $W \ge 0$. To keep the notation concise, we'll often write W instead of $W|_{B_n}$, in the sequel.

2.1. PROPOSITION. Let H and \tilde{H}_n , $n \ge n_0$, be as above, and let $E \in (a, b)$. Assume that W is a non-negative, bounded function, tending to 0 at infinity. We then have

$$N_{\pm}(\lambda; H - E, W) \ge \limsup_{n \to \infty} N_{\pm}(\lambda'; \tilde{H}_n - E, W|_{B_n}), \quad 0 < \lambda' < \lambda, \qquad (2.1)$$

$$N_{\pm}(\lambda; H - E, W) \le \liminf_{n \to \infty} N_{\pm}(\lambda'; \tilde{H}_n - E, W|_{B_n}), \quad 0 < \lambda < \lambda'.$$
(2.2)