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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 $W \geq 0$ 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

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

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

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 $W = W_+ - W_-$, $W_\pm \geq 0$.

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 $\mathbf{R}^\nu$. $N_-(\infty; K)$ 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 W is 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.

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 $\sigma_{\text{ess}}(H)$, 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 $\mathbf{R}^\nu$, 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

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

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

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

Here the important point is that $\tilde{H}_n$ has a spectral gap containing the interval $[a, b]$, for sufficiently large n, i. e.,

$$\sigma(\tilde{H}_n) \cap [a, b] = \emptyset, \quad n \geq n_0.$$

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 $W \geq 0$. To keep the notation concise, we'll often write W instead of $W|_{B_n}$, in the sequel.

2.1. PROPOSITION. *Let H and $\tilde{H}_n$, $n \geq n_0$, 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*

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

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

By this approximation process, we have gained the following: as the operators $\tilde{H}_n - \mu W$ all have compact resolvent, we can count eigenvalues starting from the bottom of the spectrum. From Kato-Rellich perturbation theory it is then clear that

$$N_+(\lambda; \tilde{H}_n - E, W) = \dim P_{(-\infty,E)}\left(\tilde{H}_n\right) - \dim P_{(-\infty,E)}\left(\tilde{H}_n - \lambda W\right),$$

and similarly for N_-. Therefore, we can obtain information on $N_{\pm}(\lambda; \tilde{H}_n - E, W)$ by simply counting how many eigenvalues have been moved over the level E by the perturbation λW. Here we use the notation "$\dim P_{(-\infty,E)}(.)$" to denote the number of eigenvalues below E, counting multiplicities.

By a different method, one can prove the following convergence result for the case $W = W_+ - W_-$ (note that we do *not* get an upper bound here).

2.2. PROPOSITION. (cf. [15; Proposition 2.4])*Let H and $\tilde{H}_n$, $n \geq n_0$, be as above, and let $E \in (a,b)$. Suppose that W is a bounded function tending to zero at infinity. Then, for $0 < \lambda < \lambda'$, we have*

$$N_{\pm}(\lambda'; H - E, W) \geq \limsup_{n \to \infty} \left| \dim P_{(-\infty,E)}\left(\tilde{H}_n\right) - \dim P_{(-\infty,E)}\left(\tilde{H}_n \mp \lambda W\right) \right|.$$

The above approximation scheme has simplified the problem, but the eigenvalue counting for $\tilde{H}_n$ and $\tilde{H}_n - \lambda W$ is by no means trivial. As a second main step in the proof, we use decoupling inside the ball B_n to separate the region where λW is active from the region where λW may be neglected. As W decays, this will in particular ensure that the interaction between W and the non-local operator $\psi_n \Pi_n \psi_n$ will be negligable. To obtain upper or lower bounds, we decouple by means of a DBC or NBC on ∂B_R, where the radius R is chosen in such a way that W is sufficiently small outside B_R; note that this can be done independently of n, at least for n large. Here our basic lemma reads as follows ($\mathcal{B}_p$ denotes the p-th Schatten ideal or trace ideal, for $1 \leq p < \infty$; cf. Simon [25]):

2.3. LEMMA. (*cf.* [15; Proposition 1.3]) *Let A, B be compact, symmetric operators and suppose that $B \in \mathcal{B}_p$, for some $p \in [1, \infty)$. Also let $\eta > 0$, $\eta \in \rho(A)$. Then*

$$\left| \dim P_{(\eta,\infty)}(A) - \dim P_{(\eta,\infty)}(A + B) \right| \leq \left\| (A - \eta)^{-1} \right\|^p \cdot \|B\|^p_{\mathcal{B}_p},$$

where $\dim P_{(\eta,\infty)}$ counts the eigenvalues in (η, ∞), repeated according to their multiplicities.

In order to apply this perturbation result in our situation, we need some more notation: Letting $-\Delta_{R;N}$ denote the Neumann Laplacian on B_R, and $-\Delta_{R,n;N,D}$ the Laplacian on the spherical shell $B_n - \bar{B}_R$, with NBC on ∂B_R and DBC on ∂B_n, we have the following trace ideal estimate:

2.4. PROPOSITION. *Let $m > 0$ and let $p > \nu/2$, $p = 2^q$, for some $q \in \mathbf{N}$. Then there exist constants $c, C > 0$ such that*

$$\left\| (-\Delta_n + m)^{-1} - (-\Delta_{R;N} \oplus -\Delta_{R,n;N,D} + m)^{-1} \right\|_{\mathcal{B}_p}^p \leq cR^{\nu-1},$$

and

$$\left\| (-\Delta_n + m)^{-1} - (0|_{B_R}) \oplus (-\Delta_{R,n;N,D} + m)^{-1} \right\|_{\mathcal{B}_p}^p \leq CR^{\nu},$$

for $1 \leq R < n$, where $0|_{B_R}$ denotes the zero operator on $L_2(B_R)$.

A proof of this basic decoupling result can be found in [15;Appendix]; of course, there is a corresponding result for DBC on ∂B_R.

While min-max methods and monotonicity imply that adding Neumann (resp., Dirichlet) boundary conditions increases (resp., decreases) the number of eigenvalues below E, we need estimates which go in the other direction. In the following proposition, we let $-\Delta_{R;N}$ denote the Neumann Laplacian on B_R, $-\Delta_{R,n;ND}$ the Laplacian on $B_n - \bar{B}_R$ with NBC on ∂B_R and DBC on ∂B_n. Then $H_{R;N}$ denotes the operator $-\Delta_{R;N} + V|_{B_R}$ while $\tilde{H}_{R,n;N,D} = -\Delta_{R,n;ND} + V|_{B_n - \bar{B}_R} + c'\psi_n \Pi_n \psi_n$, so that the direct sum $H_{R;N} \oplus \tilde{H}_{R,n;N,D}$ is nothing else but $\tilde{H}_n$ with an additional NBC on ∂B_R.

2.5. PROPOSITION. *(cf. [15; Lemma 3.2]) Let H and $\tilde{H}_n$, $n \geq n_0$, be as above and let $E' \in (a, b)$. Then, for $n \geq n_0$ and $1 \leq R \leq n/2$, we have*

$$\dim P_{(-\infty, E')}(H_{R;N}) + \dim P_{(-\infty, E')}\left(\tilde{H}_{R,n;N,D}\right)$$

$$\leq \dim P_{(-\infty, E')}\left(\tilde{H}_n\right) + CR^{\nu-1},$$

with a constant C which is independent of n and R.

To prove an estimate of this type, we apply Lemma 2.3 to the resolvents, use the second resolvent equation to get rid of the potential V and the $\psi_n \Pi_n \psi_n$-term and conclude with an application of the trace ideal estimate given in Proposition 2.4. Of course, decoupling by a DBC on ∂B_R leads to a similar estimate; in the subsequent proposition, we let $-\Delta_{R,n;D}$ denote the Dirichlet Laplacian on $B_n - \bar{B}_R$ and $\tilde{H}_{R,n;D} := -\Delta_{R,n;D} + V|_{B_n - \bar{B}_R} + c'\psi_n \Pi_n \psi_n$.

2.6. PROPOSITION. (*cf.* [15; Lemma 3.2]) *Let H and $\tilde{H}_n$, $n \geq n_0$, be as above and let $E' \in (a, b)$. Then, for $n \geq n_0$ and $1 \leq R \leq n/2$, we have*

$$\dim P_{(-\infty, E')}(H_R) + \dim P_{(-\infty, E')}\left(\tilde{H}_{R,n;D}\right) \geq \dim P_{(-\infty, E')}\left(\tilde{H}_n\right) - CR^{\nu-1},$$

with a constant C which is independent of n and R.

3. Some asymptotic bounds.

As a first illustration of our approach, we prove a simple *lower* bound for N_+ in the general case $W = W_+ - W_-$, with $W_\pm \geq 0$; note that there is now no need to consider N_- separately because this would only mean to switch from W to $-W$.

Here the main difficulty comes from the competition between the attractive part W_+ and the repulsive part W_- . If W_- decays faster than quadratically, then W_+ always wins over W_- (cf. [1, 15]), and we'll concentrate now on a case where W_- decays slowly,

$$W_-(x) \leq c_0(1 + |x|)^{-\alpha}, \qquad x \in \mathbf{R}^\nu, \tag{3.1}$$

for some constants $c > 0$ and $0 < \alpha \leq 2$. The following Theorem 3.1 is a refinement of Corollary 3.5 in [15], where some other related results may be found.

3.1. THEOREM. *Let H be as above, $E \in \mathbf{R} - \sigma(H)$ and suppose that W is bounded and tends to 0 at infinity, with W_- satisfying condition (3.1) for some $0 < \alpha \leq 2$. For W_+ we assume that there exist constants $k \geq 2$, $c_1, c_1' > 0$, $0 < \beta < \alpha$ and γ, where γ satisfies*

$$\nu - 1 \geq \gamma > \nu - 1 - \nu(\alpha - \beta)/2, \tag{3.2}$$

with the property that each spherical shell $B_{nk} - B_{(n-1)k}$, $n = 1, 2, \ldots$, contains at least $c_1'[n^\gamma]$ mutually disjoint balls of radius 1 on which W is bounded from below by $c_1 n^{-\beta}$.

Then there exists a positive constant C such that

$$N_+(\lambda; H - E, W) \geq C\lambda^\kappa, \quad \lambda \geq 1,$$

where $\kappa := (\nu(\alpha - \beta) + 2\gamma + 2)/2\alpha$.

PROOF. As in [1, 15], we let $E_1 := (a + E)/2$ and define

$$R = R(\lambda) = (c_0\lambda/(E - E_1))^{1/\alpha}, \quad \lambda \geq 1.$$

Then it is clear from (3.1) that $0 \leq \lambda W_-(x) \leq E - E_1$, for $|x| \geq R(\lambda)$. We now decouple by means of a DBC on ∂B_R to obtain

$$\dim P_{(-\infty,E)}(\tilde{H}_n - \lambda W)$$
$$\geq \dim P_{(-\infty,E)}(H_R - \lambda W) + \dim P_{(-\infty,E_1)}(\tilde{H}_{R,n;D}). \tag{3.3}$$

We first consider the second term on the RHS of (3.3) where Proposition 2.2 implies that

$$\dim P_{(-\infty,E_1)}(\tilde{H}_{R,n;D}) \geq \dim P_{(-\infty,E_1)}(\tilde{H}_n) - \dim P_{(-\infty,E_1)}(H_R) - c'R^{\nu-1}$$
$$= \dim P_{(-\infty,E)}(\tilde{H}_n) - \dim P_{(-\infty,E_1)}(H_R) - c'R^{\nu-1},$$

as E and E_1 belong to the same gap of $\tilde{H}_n$. For the second term on the RHS of (3.3), we introduce DBC on the boundaries of the balls where the lower bound for W holds; we discard the remaining portion of B_R. By Weyl's Law, there exist constants $c_2 > 0$ and c_3 such that

$$\dim P_{(-\infty,\mu)}(-\Delta_1) \geq c_2 \mu^{\nu/2} - c_3, \qquad \mu \geq 0,$$

and it follows that

$$\dim P_{(-\infty,E)}(-\Delta_1 + \|V\|_\infty - c_1\lambda n^{-\beta}) \geq c_4\lambda^{\nu/2}n^{-\nu\beta/2} - c_5, \qquad \lambda \geq 0.$$

Summing up the individual contributions coming from the balls of radius 1 where the lower bound for W holds, we now obtain

$$\dim P_{(-\infty,E)}(H_R - \lambda W) \geq c_5 \sum_{n \leq R/k} n^\gamma \lambda^{\nu/2} n^{-\nu\beta/2} - c_6 \text{Vol}(B_R)$$
$$\geq c_7 \lambda^{\nu/2} \lambda^{(1+\gamma-\nu\beta/2)/\alpha} - c_8 \lambda^{\nu/\alpha},$$

as $R \sim \lambda^{1/\alpha}$; also note that our assumptions imply that $\gamma - \nu\beta/2 > -1$.
Using all of the above information in the RHS of (3.3) and also the estimate

$$\dim P_{(-\infty,E_1)}(H_R) \leq c_9 \lambda^{\nu/\alpha}, \qquad \lambda \geq 1,$$

which is immediate by Weyl's Law, we finally see that

$$\dim P_{(-\infty,E)}(\tilde{H}_n - \lambda W) - \dim P_{(-\infty,E)}(\tilde{H}_n)$$
$$\geq \dim P_{(-\infty,E)}(H_R - \lambda W) - \dim P_{(-\infty,E_1)}(H_R) - c'R^{\nu-1}$$
$$\geq C_1\lambda^\kappa - C_2\lambda^{\nu/\alpha} - C_3\lambda^{\nu/\alpha} - C_4\lambda^{(\nu-1)/\alpha}$$
$$\geq C\lambda^\kappa,$$

for λ large, since $\kappa > \nu/\alpha$ for γ in the interval defined by (3.2). Now the result follows immediately via Proposition 2.2. ∎

To obtain an upper bound for $N_+(\lambda; H-E, W)$, we next try to squeeze some information from the associated (non-symmetric) Birman-Schwinger kernel.

3.2. THEOREM. *Let H be as above, and let $E \in (a, b)$. Suppose that W satisfies the decay condition*

$$|W(x)| \le c(1 + |x|)^{-\alpha}. \qquad x \in \mathbf{R}^{\nu},$$

with some positive constants c and α. Then, for any $p > \nu/\min\{\alpha, 2\}$, we have

$$\limsup_{\lambda \to \infty} \lambda^{-p} N_+(\lambda; H - E, W) < \infty.$$

PROOF. (1) Suppose $0 < \lambda_1 \le \lambda_2 \le \ldots \le \lambda_j \le \ldots$, with $\lambda_j \to \infty$, are the positive coupling constants where the kernel of $H - \lambda_j W - E$ is non-trivial, repeated according to the dimension of $\ker(H - \lambda_j W - E)$. By the Birman-Schwinger-principle, the numbers $\kappa_j := \lambda_j^{-1}$ are eigenvalues of the Birman-Schwinger kernel

$$\mathcal{K} := (\operatorname{sgn} W)|W|^{1/2}(H - E)^{-1}|W|^{1/2},$$

and (geometric) multiplicities are preserved. Now the Schur-Lalesco-Weyl theorem (*cf., e. g.,* [24, 25]) implies that

$$\sum_j \kappa_j^p \le \sum_j \mu_j^p,$$

where the μ_j denote the singular values of $\mathcal{K}$. As a consequence, we obtain the estimate

$$\left(\sum \lambda_j^{-p}\right)^{1/p} \le \|\mathcal{K}\|_{\mathcal{B}_p}.$$

We next plug in $(-\Delta + 1)^{1/2}(-\Delta + 1)^{-1/2}$ and write

$$A := (-\Delta + 1)^{1/2}(H - E)^{-1}(-\Delta + 1)^{1/2},$$

which is a bounded operator, to conclude that

$$\|\mathcal{K}\|_{\mathcal{B}_p} = \left\|W^{1/2}(-\Delta + 1)^{-1/2}A(-\Delta + 1)^{-1/2}|W|^{1/2}\right\|_{\mathcal{B}_p}$$

$$\le \left\|W^{1/2}(-\Delta + 1)^{-1/2}\right\|_{\mathcal{B}_{2p}} \cdot \|A\| \cdot \left\|(-\Delta + 1)^{-1/2}|W|^{1/2}\right\|_{\mathcal{B}_{2p}},$$

by Hölder's inequality for trace ideals ([25]). By the estimates given in [23; Theorem XI.20], it is clear that the trace-ideal norms on the RHS are finite, since, by assumption, $p > \nu/2$ and $p > \nu/\alpha$. We have therefore shown that $\sum_j \lambda_j^{-p}$ is finite, and the result follows. ∎

REMARKS. (a)Our result falls short of proving the more "natural" estimate $N_+(\lambda; H - E, W) \le c\lambda^{\nu/\min\{2,\alpha\}}$. However, in the case of W changing its sign we can't exclude that eigenvalue branches wiggle around the level E for a while which might increase the counting function considerably.

(b) The bound derived above is not only valid for positive coupling constants, but it gives as well a bound for *all* complex eigenvalues λ in the generalized eigenvalue problem $(H - E)u = \lambda W u$.

4. High barriers with compact support.

In this section, we consider $H + \lambda \chi_K$, for positive λ tending to ∞, where χ_K denotes the characteristic function of the compact set $K \subset \mathbf{R}^\nu$. It is shown in [15] that a potential barrier of the type $\lambda \chi_{B_R}$ sweeps out all the states of H having energy below E and "living" in the ball B_R, provided λ is large enough, up to an error term of order $R^{\nu-1}$. We are now trying to understand the mechanism working for compact K's which are very different from balls. Here, again, we ask for the large coupling constant limit

$$N_-(\infty; K) := \lim_{\lambda \to \infty} N_-(\lambda; H - E, \chi_K), \qquad (4.1)$$

that is, the total number of eigenvalues of $H + \lambda \chi_K$ which are shifted over the level E as λ grows from 0 to $+\infty$. Note that the quantity $N_-(\infty; K)$ is always finite if K is bounded.

Here we'll see the following mechanism at work: as λ tends to infinity, the operators $H + \lambda \chi_K$ converge in strong resolvent sense to the operator $-\Delta + V$ in the exterior domain $\mathbf{R}^\nu - K$, with DBC on ∂K. This leads to a decoupling via DBC on ∂K, and, as a consequence, the mere *volume* of the set K doesn't tell much about $N_-(\infty; K)$.

In the sequel, we shall always assume that K is a compact subset of $\mathbf{R}^\nu$ and that $R > 0$ is so large that $K \subset B_R$. Our estimates will involve two auxiliary operators defined on the domain $\Omega(R) = B_R - K$: first, we let $H_{\Omega(R);D}$ denote $-\Delta + V$, acting in $L_2(\Omega(R))$, with DBC on $\partial\Omega(R)$; second, we let $H_{\Omega(R);D,N}$ denote $-\Delta + V$ on $\Omega(R)$, with DBC on ∂K and NBC on ∂B_R. As we shall see below, the quantities relevant for the eigenvalue counting are given by

$$n_{K;N} = \dim P_{(-\infty,E)}(H_{R;N}) - \dim P_{(-\infty,E)}(H_{\Omega(R);D,N}) \qquad (4.2)$$

and

$$n_{K;D} = \dim P_{(-\infty,E)}(H_R) - \dim P_{(-\infty,E)}(H_{\Omega(R);D}). \qquad (4.3)$$

The numbers $n_{K;N}$ and $n_{K;D}$ give lower (respectively, upper) bounds for the quantity $N_-(\infty; K)$, up to an error of order $R^{\nu-1}$. This reduces the problem to the study of an explicit situation on the finite region B_R; in view of the error terms, R should be chosen as small as possible.

4.1. THEOREM. *Suppose K is a compact subset of $\mathbf{R}^\nu$ and $R \geq 1$ is such that $K \subset B_R$. With the above notation, we then have*

$$N_-(\infty; K) \geq n_{K;N} - CR^{\nu-1},$$

where the constant C is independent of K and R.

PROOF. By Proposition 2.1, it is enough to produce a lower bound

$$\sup_{\lambda>0} N_-(\lambda; \tilde{H}_n - E, \chi_K) \geq n_{K;N} - CR^{\nu-1}, \tag{4.4}$$

for n large. Without restriction, we may assume that E is not an eigenvalue of $H_{\Omega(R);D,N}$. Introducing NBCs on ∂B_R, monotonicity of the associated quadratic forms implies that

$$\dim P_{(-\infty,E)}(\tilde{H}_n + \mu\chi_K)$$
$$\leq \dim P_{(-\infty,E)}\left(\tilde{H}_{R,n;N,D}\right) + \dim P_{(-\infty,E)}\left(H_{R;N} + \mu\chi_K\right)$$
$$\leq \dim P_{(-\infty,E)}\left(\tilde{H}_n\right) - \dim P_{(-\infty,E)}\left(H_{R;N}\right) + CR^{\nu-1}$$
$$+ \dim P_{(-\infty,E)}\left(H_{R;N} + \mu\chi_K\right),$$

by Proposition 2.5, whence

$$\dim P_{(-\infty,E)}\left(\tilde{H}_n\right) - \dim P_{(-\infty,E)}\left(\tilde{H}_n + \mu\chi_K\right)$$
$$\geq \dim P_{(-\infty,E)}\left(H_{R;N}\right) - \dim P_{(-\infty,E)}\left(H_{R;N} + \mu\chi_K\right) - CR^{\nu-1}. \tag{4.5}$$

By classical convergence results for eigenvalues (cf. Simon [26], Weidmann [27]), the eigenvalues of $H_{R;N} + \mu\chi_K$ increase monotonically to the corresponding eigenvalues of $H_{\Omega(R);D,N}$, as $\mu \to \infty$. Taking into account the definition of $n_{K;N}$, we have therefore shown that the LHS of (4.5) is eventually greater or equal to $n_{K;N} - CR^{\nu-1}$, for $\mu \to \infty$. By Kato–Rellich perturbation theory, this implies (4.4), and we are done. ∎

REMARK. The decoupling effect becomes most visible if K has lots of holes which are so small that the Dirichlet Laplacian on each hole has no eigenvalue below E ("swiss cheese"). In this case, we see that $n_{K;N} = n_{\tilde{K};N}$, where $\tilde{K}$

is obtained from K by taking the union of K with all bounded components of $\mathbf{R}^\nu - K$. For example, it is possible to have $\hat{K} = B_R$ while the volume of K itself is arbitrarily small.

In $\mathbf{R}^\nu$, $\nu \geq 2$, the opposite situation is also possible. In fact, it is easy to construct examples where K has large volume while *no* eigenvalues cross E (think of K as a union of many small balls which are well separated; cf. [13, 1]).

The corresponding upper bound is somewhat easier.

4.2. THEOREM. *Suppose K is a compact subset of $\mathbf{R}^\nu$ and $R \geq 1$ is such that $K \subset B_R$. With the above notation, we then have*

$$N_-(\infty; K) \leq n_{K;D} + CR^{\nu-1},$$

where the constant C is independent of K and R.

PROOF. Proceeding as in the proof of the lower bound, we now use Dirichlet decoupling on ∂B_R and Proposition 2.6 to obtain

$$\dim P_{(-\infty, E)}\left(\tilde{H}_n\right) - \dim P_{(-\infty, E)}\left(\tilde{H}_n + \mu \chi_K\right)$$
$$\leq \dim P_{(-\infty, E)}\left(H_R\right) - \dim P_{(-\infty, E)}\left(H_R + \mu \chi_K\right) + CR^{\nu-1}$$
$$\leq n_{K;D} + CR^{\nu-1}, \qquad \mu > 0, \quad n \geq n_0,$$

by monotonicity and the definition of $n_{K;D}$. By Kato–Rellich perturbation theory, this implies that $N_-(\mu; \tilde{H}_n - E, \chi_K) \leq n_{K;D} + CR^{\nu-1}$, for n large, and the desired result follows via Proposition 2.1. ∎

REMARK. It is clear that one can use the standard techniques of Dirichlet–Neumann bracketing in order to derive (crude) estimates for $n_{K;D}$ in concrete situations, but sharp information on $n_{K;D}$ may be difficult to obtain (cf. also Kirsch [17]). An even more challenging problem consists in finding bounds for $n_{K;N} - n_{K;D}$.

References.

[1] S. Alama, P. A. Deift and R. Hempel: Eigenvalue branches of the Schrödinger operator $H - \lambda W$ in a spectral gap of H. Commun. Math. Phys. **121** (1989), 291-321.

[2] S. Alama and Y.Y. Li: Existence of solutions for semilinear elliptic equations with indefinite linear part. Preprint, 1990.

[3] N. W. Ashcroft and N. D. Mermin: *Solid State Physics.* Holt, Rinehart and Winston, New York 1976.

[4] M. Sh. Birman: Discrete spectrum in the gaps of the continuous one in the large coupling constant limit. In: *Operator Theory: Advance and Applications*, Vol. 46. Birkhäuser, Basel 1990.

[5] Ph. Briet, J. M. Combes and P. Duclos: Spectral stability under tunneling. Commun. Math. Phys. **126** (1989), 133-156.

[6] R. Courant and D. Hilbert: *Methods of Mathematical Physics.* Vol. I. Interscience, New York 1953.

[7] P. A. Deift and R. Hempel: On the existence of eigenvalues of the Schrödinger operator $H - \lambda W$ in a gap of $\sigma(H)$. Commun. Math. Phys. **103** (1986), 461-490.

[8] P. A. Deift and B. Simon: On the decoupling of finite singularities from the question of asymptotic completeness in two-body quantum systems. J. Funct. Anal. **23** (1976), 218-238.

[9] M. S. P. Eastham:*The spectral theory of periodic differential equations.* Scottish Academic Press, Edinburgh 1973.

[10] F. Gesztesy, D. Gurarie, H. Holden, M. Klaus, L. Sadun, B. Simon and P. Vogl: Trapping and cascading of eigenvalues in the large coupling limit. Commun. Math. Phys. **116** (1988), 597-634.

[11] F. Gesztesy and B. Simon: On a theorem of Deift and Hempel. Commun. Math. Phys. **116** (1988), 503-505.

[12] I. C. Gohberg and M. G. Krein: *Introduction to the Theory of Linear Nonselfadjoint Operators.* Amer. Math. Soc., Providence (R. I.) 1969.

[13] R. Hempel: *A left-indefinite generalized eigenvalue problem for Schrödinger operators.* Habilitationsschrift, Univ. München 1987.

[14] R. Hempel: On the asymptotic distribution of the eigenvalue branches of the Schrödinger operator $H + \lambda W$ in a spectral gap of H. J. Reine Angew. Math. **399** (1989), 38-59.

[15] R. Hempel: Eigenvalues in gaps and decoupling by Neumann boundary conditions. J. Math. Anal. Appl., to appear.

[16] T. Kato: *Perturbation theory for linear operators.* Springer, New York 1966.

[17] W. Kirsch: Small perturbations and the eigenvalues of the Laplacian on large bounded domains. Proc. Amer. Math. Soc. **101** (1987), 509-512.

[18] M. Klaus: Some applications of the Birman-Schwinger principle. Helv. Phys. Acta **55** (1982), 49-68.

[19] F. Klopp: Impuretés dans une structure périodique. *Journées "Equations aux dérivés partielles"* (Saint Jean des Monts, 1990), Exp. No. XX, Ecole Polytech., Palaiseau, 1990

[20] A. Outassourt: Comportement semi-classique pour l'opérateur de Schrö-
dinger à potentiel périodique. J. Funct. Anal. **72** (1987), 65-93.

[21] S.T. Pantelides: The electronic structure of impurities and other point
defects in semiconductors. Rev. Mod. Phys. **50** (1978), 797-858.

[22] M. Reed and B. Simon: *Methods of modern mathematical physics.* Vol. I.
Functional Analysis. Revised and enlarged ed. Academic Press, New York
1981.

[23] M. Reed and B. Simon: *Methods of modern mathematical physics.* Vol. III.
Scattering theory. Academic Press, New York 1979.

[24] M. Reed and B. Simon: *Methods of modern mathematical physics.* Vol.
IV.*Analysis of operators.* Academic Press, New York 1978.

[25] B. Simon:*Trace Ideals and their applications.* Cambridge Univ. Press,
London 1979.

[26] B. Simon: A canonical decomposition for quadratic forms with application
to monotone convergence theorems. J. Funct. Anal. **28** (1978), 377-385.

[27] J. Weidmann: Stetige Abhängigkeit der Eigenwerte und Eigenfunktionen
elliptischer Differentialoperatoren vom Gebiet. Math. Scand. **54**(1984), 51-
69.

[28] A. V. Sobolev: The Weyl asymptotics for discrete spectrum of the per-
turbed Hill operator. Preprint, 1991

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