Weakly coupled states on branching graphs Pavel

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exner@ujf.cas.cz **Abstract.** We consider a Schrödinger particle on a graph consisting of N

links joined at a single point. Each link supports a real locally integrable potential V_j ; the self–adjointness is ensured by the δ type boundary condition at the vertex. If all the links are semiinfinite and ideally coupled, the potential decays as $x^{-1-\epsilon}$ along each of them, is non–repulsive in the mean and weak enough, the corresponding Schrödinger operator has a single negative eigenvalue; we find its asymptotic behavior. We also derive a bound on the number of bound states and explain how the δ coupling constant may be interpreted in terms of a family of squeezed potentials.progress in investigation of "mesoscopic"

systems attracted a wave of attention to properties of quantum mechanical particles whose motion is confined to a graph — see[Ad, AL, ARZ, BT, EŠ, GPS, GLRT, GP] and references therein. Theproblem is not new; it appeared for the first time in early fifties in connection with the free–electron model of organic molecules [RuS]. However, the mentioned studies brought not only physical applications but fresh mathematical insights as well.They concern, in particular, relations between spectral properties and the dimensionality of the configuration space. For instance, band structure of the spectrum for a periodic rectangular–lattice graph exhibits an interesting dependence on number–theoretic properties of the ratio θ of the rectangle sides [E2, E3, EG]. For most values of θ there are infinitely many gaps once the the "coupling constant" at graph vertices is nonzero; hence such systems do not conform with the Bethe–Sommerfeld conjecture[Sk1, Sk2] and behave rather as one–dimensional ones. On theother hand, for a "bad–irrational" lattice there are no gaps if the coupling at the vertices is weak enough which is *not* a typical one–dimensional behavior; infinitely many gaps open only above a certain critical value.In the present letter we are going to show that the mentioned one–dimensional feature is contained already in the way in which the wavefunctions are coupled at graph vertices as long as the number of links entering a vertex is finite. In fact, we shall demonstrate that *continuous* Schrödinger operators on graphs may be regarded as an extension of the standard Sturm–Liouville theory of second–order ODE's.For simplicity, we restrict ourselves to the simplest situation of a graph with a single vertex in which a finite number of $N \geq 2$ links of lengths ℓ_j , $j = 1, \dots, N$ are joined. Since each link can be mapped to a finite or semiinfinite interval, the corresponding state Hilbert space is identified with $\mathcal{H} := \bigoplus_{j=1}^N L^2(0, \ell_j)$. We suppose that the jth–link supports a real–valued potential V_j and assume that

(p1) $V_j \in L^1_{loc}(0, \ell_j)$, $j = 1, \dots, N$,

(p2) if a given link is semiinfinite, the differentialexpression $-\frac{d^2}{dx^2} + V_j(x)$ is LPC at infinity; if $\ell_j < \infty$ this requirement is replaced by a fixed boundary condition, $\psi(\ell_j)\cos\omega_j + \psi'(\ell_j)\sin\omega_j = 0$.

Given a family $V := \{V_j\}_{j=1}^N$ and $\alpha \in I\!\!R \cup \{\infty\}$, we define the operator $H_\alpha(V)$ by

$$H_\alpha(V)\{\psi_j\} := \{-\psi_j'' + V_j\psi_j\} \tag{1}$$

with the natural domain requirements at each link and the boundary conditions

$$\psi_1 = \cdots = \psi_n =: \psi \,, \qquad \sum_{j=1}^N \psi_j' = \alpha\psi \tag{2}$$

at the vertex, where $\psi_j := \lim_{x\to 0+} \psi_j(x)$ and $\psi_j' := \lim_{x\to 0+} \psi_j'(x)$ are the corresponding boundary values. For $\alpha = \infty$ the requirement (2) is replaced by the Dirichlet condition, $\psi_j = 0$, $j = 1, \dots, N$; in that case the operator is decoupled, $H_\infty(V) = \bigoplus_{j=1}^N h_j(V_j)$. The condition (2) is known to produce a self–adjoint operator if $V = 0$ [EŠ]; it is straightforward to check that under the stated assumptions this conclusion is not changed:

Proposition 1 *The operator $H_\alpha(V)$ is self–adjoint for any $\alpha \in I\!\!R \cup \{\infty\}$ and V obeying the conditions (p1,2).*

Our first result consists of showing that if the coupling is ideal, $\alpha = 0$, and all the links are semiinfinite, an arbitrarily weak potential potential which is not repulsive in the mean and decays fast enough produces a bound state.

Theorem 2 *Let $\ell_j = \infty$ and $V_j \in L^2(I\!\!R_+, (1+|x|)dx)$, $j = 1, \dots, N$. Then the operator $H_0(\lambda V)$ has for all sufficiently small $\lambda > 0$ a single negative eigenvalue $\epsilon(\lambda) = -\kappa(\lambda)^2$ iff*

$$\sum_{j=1}^N \int_0^\infty V_j(x)\, dx \,\leq\, 0 \,. \tag{3}$$

In that case, its asymptotic behavior is given by

$$\begin{aligned}\kappa(\lambda) \;=\; -\frac{\lambda}{N} \sum_{j=1}^N \int_0^\infty V_j(x)\, dx \,-\, \frac{\lambda^2}{2N} \Bigg\{ \sum_{j=1}^N \int_0^\infty \int_0^\infty V_j(x)|x-y|V_j(y)\, dx\, dy \\ +\; \sum_{j,\ell=1}^N \left(\frac{2}{N} - \delta_{j\ell}\right) \int_0^\infty \int_0^\infty V_j(x)(x+y)V_\ell(y)\, dx\, dy \Bigg\} + \mathcal{O}(\lambda^3) \,.\end{aligned} \tag{4}$$

Under the assumptions, the essential spectrum of the Dirichlet link operators $h_j(V_j)$ is $[0,\infty)$. As we shall show below, $H_\alpha(V)$ and $H_\infty(V)$ differ by a rank–one perturbation in the resolvent, hence we have also $\sigma_{ess}(H_\alpha(V)) = [0,\infty)$. Moreover, the operators $h_j(\lambda V_j)$ have no discrete spectrum for small λ, so $H_\alpha(\lambda V)$ has at most one negative eigenvalue.To prove the existence condition (3) and the asymptotic expansion (4), we employ the explicit form of the resolvent; we shall derive it for the general case. Denote $H_\alpha := H_\alpha(V)$. Given k with $\mathrm{Im}\, k \ge 0$, $k^2 \in \rho(H_\infty)$, we denote by $u_j \equiv u_j(\cdot;k)$ and $v_j \equiv v_j(\cdot;k)$ solutions to $-\psi_j'' + V_j\psi_j = k^2\psi_j$ with the appropriate behavior at 0 and ℓ_j, respectively, *i.e.*, $u_j(0;k) = 0$ while v_j is square integrable at infinity if $\ell_j = \infty$ and satisfies the fixed boundary condition otherwise. If $\alpha = \infty$, the links are decoupled and the corresponding components of H_∞ are characterized by the resolvent kernels

$$g_j(x,y;k) := -\frac{u_j(x_<;k)v_j(x_>;k)}{W(u_j,v_j)}, \tag{5}$$

where conventionally $x_< := \min\{x,y\}$ and similarly for $x_>$, and $W(u_j,v_j)$ is the Wronskian of the two solutions.

Lemma 3 *Assume (p1,2). For arbitrary* $\alpha \in I\!\!R$ *and* k *such that* $\mathrm{Im}\, k \ge 0$ *and* $k^2 \in \rho(H_\infty) \cap \rho(H_\alpha)$, *the resolvent* $(H_\alpha - k^2)^{-1}$ *is amatrix integral operator with the kernel*

$$G^\alpha_{j\ell}(x,y;k) = \delta_{j\ell}g_j(x,y;k) + \frac{v_j(x;k)v_\ell(y;k)}{v_j(0;k)v_\ell(0;k)(\alpha - M(k))}, \tag{6}$$

where $M(k) := \sum_{j=1}^N \frac{v_j'(0;k)}{v_j(0;k)}$.

Proof: By Krein's formula [AGHH, Appendix A], the sought kernel is of the form $\delta_{j\ell}g_j(x,y;k) + \Lambda_{j\ell}v_j(x;k)v_\ell(y;k)$. To find the unknown coefficients, we express from here $\psi := (H_\alpha - k^2)^{-1}\phi$. Since ψ has to satisfy the boundary conditions (2) for any $\phi \in \mathcal{H}$, we arrive at a system of linear equations for $\Lambda_{j\ell}$ which yields (6). ∎

Remark 4 Eigenvalues of $H_\alpha(V)$ are determined by zeros of the denominator in (6). Since all the logarithmic derivatives are decreasing functions of k, so is $M(k)$, and each interval between neigbouring points of $\bigcup_{j=1}^N \sigma_{disc}(h_j(V_j))$ contains for an arbitrary $\alpha \in I\!\!R$ just one simple eigenvalue. Hence the multiplicity of $\sigma_{disc}(H_\alpha(V))$ in the coupled case, $\alpha \ne \infty$, does not exceed $N-1$; in particular, the discrete spectrum is simple for $N = 2$. On the other hand, eigenvalues of multiplicity $N-1$ arise naturally if $H_\infty(V)$ has a "fully degenerate" eigenvalue as noticed in [GPS].

Proof of Theorem 2: We have $H_0(\lambda V) = A_0 + \lambda V$, where $A_0 := H_0(0)$. The well–known resolvent formula [AGHH, Appendix B] shows that possible negative eigenvalues of $H_0(\lambda V)$ are given by the Birman–Schwinger principle: such an eigenvalue exists *iff* λK has the eigenvalue -1, where $K := |V|^{1/2}(A_0 - k^2)^{-1}V^{1/2}$ is determined by its kernel,

$$
\begin{aligned}
K_{j\ell}(x,y;k) \;&:=\; \delta_{j\ell}|V_j(x)|^{1/2}\,\frac{\sinh \kappa x_< \, e^{-\kappa x_>}}{\kappa}\, V_j(y)^{1/2} \\
&+\; \frac{1}{\kappa N}\,|V_j(x)|^{1/2} e^{-\kappa(x+y)} V_\ell(y)^{1/2}\,,
\end{aligned}
\tag{7}
$$

where we have introduced $\kappa := -ik$ and $V_j(\cdot)^{1/2}$ is the standard signed square root of the potential. Writing $K = P_\kappa + Q_\kappa$, we find that the first part can be estimated as

$$
\|P_\kappa\|^2 \;\le\; \|P_\kappa\|_{HS}^2 \;\le\; \sum_{j=1}^N \int_0^\infty \int_0^\infty |V_j(x)| x_<^2 |V_j(y)|\, dx\, dy \;\le\; \sum_{j=1}^N \left(\int_0^\infty x|V_j(x)|\, dx \right)^2,
$$

so it has a bound independent of κ and the operator P_0 corresponding to the kernel $P_{0,j\ell}(x,y;k) := \delta_{j\ell} V_j(x)\, x_<^2 V_j(y)$ is well–defined.Furthermore, Q_κ is rank–one and the same is true for

$$
\lambda(I+\lambda P_\kappa)^{-1} Q_\kappa \;=\; (\psi,\cdot)\phi\,,
\tag{8}
$$

where

$$
\psi \;:=\; \frac{\lambda}{\kappa N}\, e^{-\kappa\cdot} V^{1/2}\,, \quad \phi \;:=\; (I+\lambda P_\kappa)^{-1} e^{-\kappa\cdot} |V|^{1/2}\,;
$$

due to the above result the inverse makes sense for all λ small enough. Using the identity

$$
(I+\lambda K)^{-1} \;=\; [I+\lambda(I+\lambda P_\kappa)^{-1} Q_\kappa]^{-1} (I+\lambda P_\kappa)^{-1}
$$

we find that for small λ eigenvalues of λK coincide with those of the operator (8). However, the latter has just one eigenvalue $\xi(\lambda) = (\psi,\phi)$. Demanding $\xi(\lambda) = -1$ we get an implicit equation for $\kappa(\lambda)$; the rest of the argument is the same as in[BGS, Kl]. If the potential mean (3) equals zero, the linear term is absent as well as the $2/N$ part of the quadratic one, so

$$
\kappa(\lambda) \;=\; -\,\frac{\lambda^2}{4N} \sum_{j=1}^N \int_{\mathbb{R}^2} \tilde V_j(x)\, |x-y| \tilde V_j(y)\, dx\, dy \;+\; \mathcal{O}(\lambda^3)\,,
$$

where $\tilde V_j$ is the odd extension of V_j to the whole $\mathbb{R}$; hence the standard argument works again. $\blacksquare$ In the case $N=2$ the asymtotic expansion (4) reduces to the well–known formula for Schrödinger operators on line [BGS, Kl]; the present proof illustrates why the factorization of the singular part in these papers (in contrast to [Si]) was optimal. In the same way one can generalize the trace–class bound on the number of one–dimensional Schrödinger operators [Se, Kl, Ne].

Proposition 5 *Let $\ell_j = \infty$ and $V_j^{(-)} := \max\{0, -V_j\} \in L^2(\mathbb{R}_+, (1+|x|)dx)$ for $j = 1,\dots,N$. Then the number of negative eigenvalues of $H_0(V)$ may be estimated* *by*

$$N(V^{(-)}) \;\le\; 1 + \frac{1}{2\langle V^{(-)}\rangle} \left\{ \sum_{j=1}^{N} \int_0^\infty \int_0^\infty |x-y|\, V_j^{(-)}(x) V_j^{(-)}(y)\, dx\, dy \right.$$
$$\left. + \sum_{j,\ell=1}^{N} \left(\frac{2}{N} - \delta_{j\ell} \right) \int_0^\infty \int_0^\infty (x+y)\, V_j^{(-)}(x) V_\ell^{(-)}(y)\, dx\, dy \right\}, \tag{9}$$

where $\langle V^{(-)}\rangle := \sum_{j=1}^N \int_0^\infty V_j^{(-)}(x)\, dx$.

It is well known that the δ interaction on line can be approximated by means of a family of squeezed potentials. In the present context we can extend this result to branching graphs; this gives the boundary condition (2) with a nonzero α a natural meaning of low–energy description of a non–ideal junction. Given W_j we define the scaled potentials by

$$W_{\epsilon,j} := \frac{1}{\epsilon} W_j \left(\frac{x}{\epsilon} \right), \quad j = 1, \dots, N\,. \tag{10}$$

Theorem 6 *Suppose that* $V_j \in L^1_{loc}(0,\ell_j)$ *are below bounded and* $W_j \in L^1(0,\ell_j)$ *for* $j = 1,\dots,N$ *. Then*

$$H_0(V+W_\epsilon) \longrightarrow H_\alpha(V) \qquad \text{as} \quad \epsilon \to 0+ \tag{11}$$

in the norm resolvent sense, where $\alpha = \langle W\rangle := \sum_{j=1}^N \int_0^\infty W_j(x)\, dx$.

Proof: Let $G^{W_\epsilon}_{j\ell}(x,y;k)$ denote the resolvent kernel of $H_0(V+W_\epsilon)$. Using once more the resolvent formula, we may rewrite it as

$$\begin{aligned} G^{W_\epsilon}_{j\ell}(x,y;k) \;&=\; G^0_{j\ell}(x,y;k) - \sum_{r,s} \int_0^\infty \int_0^\infty G^0_{j\ell}(x,y';k)\, W_{\epsilon,r}(x')^{1/2} \\ &\times \left(I + |W_\epsilon|^{1/2} \left(H_0(V) - k^2 \right)^{-1} W_\epsilon^{1/2} \right)^{-1}_{rs} (x',x'')\, |W_{\epsilon,r}(x'')|^{1/2} \\ &\times G^0_{s\ell}(x'',y;k)\, dx'\, dx''\,. \end{aligned}$$

Changing the integration variables to x'/ϵ and x''/ϵ as in [AGHH, Sec.I.3.2], we can rewrite the resolvent in question in the form $-B_{k,\epsilon} \left(I + C_{k,\epsilon} \right)^{-1} \tilde B_{k,\epsilon}$,where the involved operators are determined by their kernels,

$$\begin{aligned} (B_{k,\epsilon})_{j\ell}(x,y) \;&=\; G^0_{j\ell}(x,\epsilon y;k) W_\ell(y)^{1/2}\,, \\ (\tilde B_{k,\epsilon})_{j\ell}(x,y) \;&=\; |W_j(x)|^{1/2} G^0_{j\ell}(\epsilon x,y;k)\,, \\ (C_{k,\epsilon})_{j\ell}(x,y) \;&=\; |W_j(x)|^{1/2} G^0_{j\ell}(\epsilon x,\epsilon y;k)\, W_\ell(y)^{1/2}\,, \end{aligned}$$

which converge pointwise to

$$\begin{aligned}(B_k)_{j\ell}(x,y) &= G^0_{j\ell}(x,0;k)W_\ell(y)^{1/2}\,,\\ (\tilde{B}_k)_{j\ell}(x,y) &= |W_j(x)|^{1/2}G^0_{j\ell}(0,y;k)\,,\\ (C_k)_{j\ell}(x,y) &= |W_j(x)|^{1/2}G^0_{j\ell}(0,0;k)\,W_\ell(y)^{1/2}\,,\end{aligned}$$

respectively, as $\epsilon\to 0+$. The explicit form of the last operator makes it possible to find the inverse,

$$(I+C_k)^{-1}_{j\ell}(x,y) \;=\; \delta(x-y)\delta_{j\ell} \,-\, \frac{|W_j(x)|^{1/2}W_\ell(y)^{1/2}}{\langle W\rangle - M(k)}\,,$$

where we have employed (6). The correction to the "free" resolvent kernel is therefore equal to

$$\begin{aligned}&-\sum_r \int_0^\infty dx'\,W_r(x')\,G^0_{jr}(x,0;k)G^0_{r\ell}(0,y;k)\\ &+\sum_{r,s}\int_0^\infty\int_0^\infty dx'\,dx''\,W_r(x')W_s(x'')\,\frac{G^0_{jr}(x,0;k)G^0_{r\ell}(0,y;k)}{\langle W\rangle - M(k)}\\ &= \frac{v_j(x;k)v_\ell(y;k)}{v_j(0;k)v_\ell(0;k)}\,\frac{\langle W\rangle}{M(k)(\langle W\rangle - M(k))}\,;\end{aligned}$$

this coincides with the analogous term in (6) if we set $\alpha:=\langle W\rangle$. It is sufficient to check the norm–resolvent convergence for a particular k. Since all the $h_j(V_j)$ are below bounded by assumption, one may choose κ large enough to get exponentially decaying solutions $v_j(\cdot;k)$ at the semiinfinite links; the argument then proceeds as in [AGHH, Sec.I.3.2]. ▮*Acknowledgments.* The author is grateful for the hospitality extended to him in the Centre de Physique Théorique, C.N.R.S., Marseille–Luminy, where this work was done. The research has been partially supported by the Grant AS No.148409.

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