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Abstract. We analyse the problem of one-dimensional quantum mechanics on arbitrary graphs as idealized models for quantum systems on spaces with non-trivial topologies. In particular we argue that such models can be made to accommodate the physical characteristics of wavefunctions on a network of wires and offer several derivations of a particular junction condition. Throughout we adopt a continuity condition for the wavefunction at each primitive node in the network. Results are applied to the problem of the energy spectrum of a system containing one and infinitely many junctions.

1. Introduction

Quantum mechanics on networks of one-dimensional wires connected at nodes has been studied recently, either as a theoretical problem in its own right [1–3] or as a means of modelling mesoscopic solid-state systems [4, 5]. The behaviour of the wavefunction at a node in a network of such wires is crucial to the determination of the energy spectrum and hence the physical behaviour of such a system. Most authors require Sturm–Liouville-type boundary condition to conserve probability flux at each node, although there is less agreement over whether the wavefunction should also be continuous there.

Ruedenberg and Scherr [6] and very recently Avishai and Land [1] are amongst those who argue that continuity must be satisfied (A good review of the work up to 1988 is provided in sections III and IV of [7]). Exner and Šeba [2, 3] leave open the question of continuity, while Shapiro and others [8–10] have analysed such systems using a beam splitter that destroys continuity.

Wavefunction continuity and flux conservation alone are not sufficient to completely specify the properties of the wavefunction at a junction. Exner and Šeba [3], using the Von Neumann theory of self-adjoint extensions of formal differential operators, have classified the various boundary conditions at a junction, while Kowal *et al* have examined the general form of the S-matrix for a beam splitter [11].

In this paper we show that the assumption of wavefunction continuity at a node leads to a junction scattering matrix which is completely specified by a single, real, energy-dependent parameter, consistent with the findings of [3]. For such a junction condition, we show that the spectrum of a particle confined to a star-shaped region consisting of M wires joined at a single node with fixed end boundary conditions can be written in terms of this parameter. We further identify a recent result of Avishai and Luck [1] for the dispersion curve of an infinite array of 1D wires as a special case of the above parametrization and generalize their result to an arbitrary junction, with wavefunction continuity.

2. Properties of junctions

Since we are interested in modelling particles confined to regions of space of arbitrary shape, we first discuss the hierarchy of approximations which we assume in order to render such a problem tractable. Our first assumption is to suppose that the confining forces arise as a result of a common uniform potential within each wire and that the surface of each wire coincides with a region where the potential experiences a sudden discontinuity. Thus the problem is simplified to that of solving for the stationary quantum states of a particle in a domain where such a potential is constant. Consider first the equation in a finite segment of such a wire. Although the wire may have curvature and torsion in space it is possible to express the Laplacian operator that features in the Schrödinger equation in terms of a coordinate system defined by a moving (Frenet) frame centered on the curve whose locus defines the centroid of the wire. In such a coordinate system the wavefunction must accommodate the inertial forces induced by the contortions of the segment in space. However if the locus of the centroid of the wire has negligible extrinsic curvature and torsion over its length the Schrödinger equation can be made separable by passing to a non-inertial frame. In such an adapted coordinate system [12] the equation is the same as that for a free particle confined to a right cylindrical segment of space. Our next hypothesis is to concentrate our attention on the longitudinal behaviour of the wavefunction defined by the locus of the centroid of the cylinder. Thus we shall assume that the wavefunction is independent of radial and azimuthal coordinates within each right-cylindrical domain. For states with this symmetry the three-dimensional Laplacian reduces effectively to a one-dimensional one. Consequently the Schrödinger equation reduces to a one-dimensional ordinary differential equation defined along the locus of the centroid. We shall persist with this truncation of the problem even in the vicinity of any junction between domains, where the untruncated problem becomes intractable. We are now in a position to model the junction conditions between different domains in terms of the behaviour of the truncated wavefunctions at the intersection of the loci of the various centroids. Similarly at any free ends of segments we may confine the particle by standard one-dimensional end-point conditions. Thus with the caveats about negligible curvatures and torsions of individual wires, and negligible wavefunction variations transverse to their longitudinal axes we have reduced the quantum mechanics of an array of coupled wires to the quantum mechanics of a particle on a graph.

With the above simplifications an eigenstate of energy $E = k^2$, in the region of a node may be written in the form

$$\psi(x, m) = A_m \exp(-\mathrm{i}kx) + B_m \exp(\mathrm{i}kx) \tag{1}$$

where (x, m) is the coordinate of a point a distance x from the node along wire m, $m = 1, \ldots, M$, with M the total number of wires connected to the node in question. Adopting the convention that $\{A_j\}$ are amplitudes of incoming plane waves and $\{B_j\}$ amplitudes of outgoing waves, the $M \times M$ scattering matrix S, associated with the node satisfies

$$|B\rangle = S|A\rangle \tag{2}$$

where $|A\rangle$ and $|B\rangle$ are the M-component column vectors, the jth components of which are respectively A_j and B_j. With this convention, S_{jj} is the reflection amplitude r_j for a particle incident on the node along wire j, while $S_{k,j\neq k}$ is the amplitude t_{kj} for such a particle to be transmitted to wire k. We now proceed by assuming that S is unitary and that the wavefunction is continuous at the node, so that

$$\lim_{x\to 0} \psi(x,m) = \psi(0) \tag{3}$$

where $\psi(0)$ is independent of m.

We first show that these assumptions imply that all the transmission amplitudes are equal and similarly all reflection amplitudes are equal. To this end consider the wavefunction $\phi_j(x,m)$ describing a wave of unit amplitude incident on the node along wire j, which satisfies

$$\begin{aligned} \phi_j(x,j) &= \exp(-\mathrm{i}kx) + r_j \exp(\mathrm{i}kx) \\ \phi_j(x, m\neq j) &= t_{mj}\exp(\mathrm{i}kx)\,. \end{aligned} \tag{4}$$

Continuity implies

$$\phi_j(0,j) = 1 + r_j = t_{1j} = \cdots = t_{j-1,j} = t_{j+1,j} = \cdots = t_{Mj}\,. \tag{5}$$

Now we consider a similar state $\phi'_j(x,m)$ describing a particle travelling out along wire j. Since $|A\rangle = S^{-1}|B\rangle = S^{\dagger}|B\rangle$, we have

$$\begin{aligned} \phi'_j(x,j) &= r_j^* \exp(-\mathrm{i}kx) + \exp(\mathrm{i}kx) \\ \phi'_j(x, m\neq j) &= t_{jm}^*\exp(-\mathrm{i}kx)\,. \end{aligned} \tag{6}$$

Hence from continuity

$$\phi'_j(0,j) = 1 + r_j^* = t_{j1}^* = \cdots = t_{j,j-1}^* = t_{j,j+1}^* = \cdots = t_{j,M}^*\,. \tag{7}$$

Expressions (5)–(7) imply that all transmission amplitudes are equal ($= t$, say) and all reflection amplitudes are equal ($= t-1 = r$, say).

To obtain expressions for r and t, one notes that unitarity of S yields

$$\begin{aligned} &|r|^2 + (M-1)|t|^2 = 1 \\ &rt^* + r^*t + (M-2)|t|^2 = 0\,. \end{aligned} \tag{8}$$

The most general solution to equations (8) with $r+1=t$ is

$$r + 1 = t = \frac{1}{M}[1 + \exp(\mathrm{i}\theta(E))] \tag{9}$$

where $\theta(E)$ is an arbitrary real function of the energy $E = k^2$ of the wavefunction.

We now examine the sum F_j defined by

$$F_j = \sum_{m=1}^{M} \left.\frac{\mathrm{d}\phi_j(x,m)}{\mathrm{d}x}\right|_{x\to 0}. \tag{10}$$

Since $F_j = \mathrm{i}k(Mt-2)$ one finds

$$\begin{aligned} \frac{F_j}{\phi_j(0,j)} &= \frac{\mathrm{i}kM(Mt-2)}{\exp(\mathrm{i}\theta(E))+1} \\ &= \mathrm{i}kM\frac{\exp(\mathrm{i}\theta(E))-1}{\exp(\mathrm{i}\theta(E))+1} \\ &= -kM\tan(\theta(E)/2)\,. \end{aligned} \tag{11}$$

Since this is valid for all j, and any eigenfunction $\psi(x,m)$ of energy E can be expressed as a linear combination of the $\phi_j(x,m)$, we find

$$\sum_{j=1}^{M} \left.\frac{\mathrm{d}\psi(x,m)}{\mathrm{d}x}\right|_{x\to 0} = V(E)\cdot\psi(0) \tag{12}$$

where $V(E) = -kM\tan(\theta(E)/2)$. It is interesting to note that for the case in which $M = 2$ and $V(E) = U$ (with U a constant), condition (12) is simply the boundary condition for a delta-potential of magnitude U.

This derivation of the junction condition in terms of stationary states involves the function $V(E)$, which encodes the detailed physical properties of the junction. In principle it may be determined by an analysis of the junction as a limit of a higher dimensional system of connected domains. Since the determination of such a limit can at best be contemplated numerically we prefer to regard $V(E)$ as a definition of the junction used to model specific situations. The simplest characterization of a junction is afforded by taking V to be an energy independent constant. We regard this as a primitive node model. A simple but important consequence is that an arbitrary graph constructed with primitive nodes (and standard free end boundary conditions on the stationary-state wavefunctions) leads to a deterministic framework for the energy spectrum of the system. A set of primitive nodes may be regarded as a complex node. Complex nodes can also be generated by dressing primitive nodes by closed loops. Each increase in complexity of a graph will be accompanied by a change in the eiegenenergy spectrum of the system. In this manner we may replace a system of junction conditions for a complex node by a single junction condition in which the primitive node coupling is renormalized to an energy dependent coupling designed to preserve the energy eigenspectrum, as described in [13]. Since the primitive node junction condition is therefore basic we shall concentrate on this aspect in the remaining sections. It is useful to note that the junction conditions for a graph constructed out of primitive nodes can also be derived from a very general variational procedure. Such a procedure is outlined in appendix A. It also follows in a non-trivial manner by a tight-binding discretization of the Schrödinger equation on a general graph (see appendix B). Both of these approaches arrive at similar conclusions by very different means and strengthen our confidence in the legitimacy and significance of condition (12).

3. Energy levels for a particle trapped near a single M-pointed junction

We now consider the dispersion relation for a network consisting of M wires each connected at one end to a common node and terminated at the other end by a standard fixed-end boundary condition. We shall call this arrangement a quantum hydra. Initially we assume the wires are all of the same length a.

To obtain the eigenstates of such a structure, consider first the travelling wave states corresponding to an incoming wave along a semi-infinite arm n. The state in arm m is written

$$\phi_n(x_m) = \begin{cases} \exp(-\mathrm{i}kx_m) + r_m \exp(\mathrm{i}kx_m) & m = n \\ t_{nm}\exp(\mathrm{i}kx_n) & m \neq n\,. \end{cases} \tag{13}$$

Energy eigenstates of system with fixed-end boundary conditions are a linear combination of the above states and in arm m take the form $\psi(x_m) = \sum_n c_n\phi_n(x_m)$. Thus with $\psi(x_m = a) = 0$ we have the M equations

$$0 = c_m(X^* + r_m X) + X\sum_{n\neq m} c_n t_{nm} \tag{14}$$

with $m = 1, \ldots, M$ and $X = \exp(\mathrm{i}ka)$. Solutions c_m exist only if $\det A = 0$, where A is the $M \times M$ matrix with elements $A_{mm} = X^* + r_m X$ and $A_{m,n\neq m} = t_{mn}X$.

For the case of a primitive junction the determinant of A factorizes as

$$\det A = [X^* + (r-t)X]^{M-1}[X^* + (r + (M-1)t)X] \tag{15}$$

$$= (X^* - X)^{M-1}(X^* + X\exp(i\theta)) \,. \tag{16}$$

Hence we immediately see that the eigenenergies are grouped into singly degenerate and $(M-1)$-degenerate levels. Solution of (16) yields $ka = n\pi$ for the degenerate levels and the transcendental equation $ka = (n+1/2)\pi - \theta/2 = (n+1/2)\pi + \tan^{-1}(V/Mk)$ for the non-degenerate levels.

We now consider the possibility of evanescent states, which, in the limit that the length of the arms tends to infinity, decay at large distances from the node. These have the form $\psi(x_m) = B\sinh\alpha(a - x_m)$, where α is an imaginary wavevector satisfying $E = -\alpha^2$, and B is a normalization constant. Substituting into (12) yields

$$\psi(0) = VA\sinh(\alpha a) = -AM\alpha\cosh(\alpha a) \tag{17}$$

from which one obtains

$$\tanh(\alpha a) = -M\alpha/V \,. \tag{18}$$

Ignoring solutions corresponding to $\alpha \leqslant 0$, since the solution with $\alpha = 0$ cannot be normalized while solutions with $\alpha < 0$ yield the same wavefunctions as those with $\alpha > 0$, we find no solutions for $V > -M/a$ and one state for $V < -M/a$. Hence for a given negative potential V there exists a critical length for the connecting wires, below which there is no negative-energy evanescent state. This analysis is readily generalized to the case where the wires have different lengths a_m, where $\psi(x_m) = (A/\sinh(\alpha a_m))\sinh(\alpha(a_m - x))$, which yields a critical potential $V = -\sum_{m=1}^{M}(1/a_m)$ above which there are no bound states. Remarkably, if just one of the connecting leads is short, then the magnitude of this critical potential remains high, even if the remaining leads become infinitely long. At first sight, this appears to contradict a standard result of scattering theory, which states that in one dimension, a negative potential of arbitrarily small magnitude induces a bound state. The reason for this difference is that the presence of the short lead effectively creates a fixed end boundary condition in the vicinity of the node, which forces ψ to vanish and reduces the effect of the scattering potential at the node.

The high degeneracy present in the eigenvalue spectrum of a hydra is of course a direct consequence of the permutation symmetry possessed by the node scattering matrix. To show that the degeneracy is lifted for structures with scattering matrices of lower symmetry, consider for example, an S-matrix of the form

$$S = \begin{pmatrix} r & T & t & t \\ T & r & t & t \\ t & t & r & T \\ t & t & T & r \end{pmatrix} . \tag{19}$$

Equation (15) remains valid, but in this case, det A becomes

$$[(X^* + (r-T)X)^2(X^* + (r + T - 2t)X)](X^* + (r + T + 2t)) \,.$$

Clearly this structure possesses a twofold degeneracy and from the form of the term in the square brackets, possesses a three-fold degeneracy in the limit $t \to T$.

As a further example we consider the following S-matrix, which is invariant under permutations of all the leads except one:

$$S = \begin{pmatrix} R & T & \cdots & T \\ T & r & \cdots & t \\ \vdots & \vdots & \ddots & \vdots \\ T & t & \cdots & r \end{pmatrix}. \tag{20}$$

This S-matrix is of particular interest, becaues for $R = 0$ it reduces to the beam splitter of Shapiro. Now we find

$$\det A = (r - t)^{M-2}[R(r + (M - 2)t) - (M - 1)T^2]$$

with an $(M - 2)$-fold degeneracy.

4. Arrays of junctions

Consider now the problem of an infinite array of junctions joined together to form a cubic lattice. For the case in which the right hand side of equation (12) is set to zero, an expression for the dispersion curve has already been obtained by Avishai and Luck [1] In this section we generalize their analysis to the case $V \neq 0$, where the right-hand side of (12) remains finite.

For a given node, let a_{n2} and b_{n2} be respectively the right-going and left-going wave amplitudes immediately to the right of the the chosen node in direction n and a_{n2} and b_{n2} be the equivalent amplitudes immediately to the right of the next node on the left. The Bloch condition then yields

$$a_{n2} = a_{n1} \exp(\mathrm{i}q_n u_n) \tag{21}$$

$$b_{n2} = b_{n1} \exp(\mathrm{i}q_n u_n) \tag{22}$$

where q_n is the component of the crystal momentum and u_n is the lattice spacing in direction n. Wavefunction continuity yields

$$f = a_{n2} + b_{n2} = a_{n1} \exp(\mathrm{i}ku_n) + b_{n1} \exp(-\mathrm{i}ku_n) \tag{23}$$

where f is a constant independent of n and k is the wavevector given by $E = k^2$, while flux conservation yields

$$\sum_{n=1}^{d} [a_{n2} - b_{n2} - a_{n1} \exp(\mathrm{i}ku_n) + b_{n2} \exp(-\mathrm{i}ku_n)] = \frac{Vf}{\mathrm{i}k}. \tag{24}$$

Solving (21)–(24) gives the relation

$$\frac{V}{k} \sin ku_n = 2 \sum_{n=1}^{d} (\cos(q_n u_n) - \cos(ku_n)). \tag{25}$$

For a cubic lattice in which the lattice constant a is the same in all directions, this yields a dispersion curve of the form

$$\cos(ka) + \frac{V}{2dk} \sin ka = \frac{1}{d} \sum_{n=1}^{d} \cos(q_n a). \tag{26}$$

When $V = 0$, equation (26) gives an explicit expression for k and hence E as a function of q, but in all other cases we have a transcendental equation that must be solved numerically.

5. Conclusion

We have motivated a particular choice of junction condition that enables one to determine the energy spectrum of a particle confined to an arbitrarily complex graph. In particular we have argued that the arbitrariness in this junction condition can be understood in terms of a renormalization of the graph topology by primitive node vertex insertions.

For networks composed of semi-infinite wires we have illustrated how amplitudes can be parametrized in analogy with the problem of scattering from a delta-function potential. We have derived the spectrum of a regular quantum hydra showing that it has a remarkably simple form, and have also generalized this to a regular array of junctions. Given the intense experimental interest in mesoscopic devices we believe our considerations may be relevant to an understanding of those properties that can be modelled in terms of quantum mechanics on graphs.

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Appendix A

In this appendix we seek to establish a variational principle that will generate Schrödinger's equation for stationary states ψ defined on an n-dimensional manifold M but in addition satisfy an appropriate boundary condition where several such manifolds join at a common junction. (An alternative derivation based on taking the limit of a tight-binding model as the distance between sites vanishes is presented in appendix B.) We write the equation in the language of exterior forms to facilitate the derivation of these conditions, giving

$$\mathrm{d} * \mathrm{d}\psi + (\mathcal{E} - \mathcal{V})\psi * 1 = 0 \tag{A1}$$

where the symbol $*$ denotes the Hodge map associated with the induced Euclidean metric on each manifold, $\mathcal{E} = \frac{2m}{\hbar^2}E$ and $\mathcal{V} = \frac{2m}{\hbar^2}V$ in terms of any potential function V and the stationary-state energy E. Thus consider a space composed of n-dimensional manifolds M_j with boundaries ∂M_j, composed by glueing together certain connected components of various boundaries.

We suppose that the stationary states on this network are extrema, for all variations of compact support, of the integral

$$\Lambda = \sum_j \Lambda_j \tag{A2}$$

where

$$\Lambda_j[\bar{\psi}_j, \psi_j] = \int_{M_j} (\mathrm{d}\bar{\psi}_j \wedge *\mathrm{d}\psi_j + \lambda_j \bar{\psi}_j \psi_j * 1) - \int_{\partial M_j} W_j \bar{\psi}_j \psi_j \omega_j \tag{A3}$$

and the sum j runs over all branches in the network. The $(n-1)$-form ω is a (Leray) measure on the junction hypersurfaces, and we have written $\lambda_j = \mathcal{V}_j - \mathcal{E}$. W_j is an arbitrary real number associated with primitive node J of the network. Taking variations of the complex field $\bar{\psi}_j$ we have

$$\mathcal{L}\Lambda_j = \int_{M_j} \mathrm{d}(\mathcal{L}\bar{\psi}_j) \wedge *\mathrm{d}\psi_j + \lambda_j(\mathcal{L}\bar{\psi}_j)\psi_j * 1 - \int_{\partial M_j} W_j(\mathcal{L}\bar{\psi}_j)\psi_j * 1 \tag{A4}$$

$$= \int_{M_j} \mathcal{L}\bar{\psi}_j(-\mathrm{d} * \mathrm{d}\psi_j + \lambda_j * \psi_j) + \int_{\partial M_j} (\mathcal{L}\bar{\psi}_j)(*\mathrm{d}\psi_j - W_j\psi_j\omega_j)\,. \tag{A5}$$

If $\mathcal{L}\bar{\psi}_j$ is a variation of compact support on the interior of the jth component space then ψ_j is extremal if

$$\mathrm{d} * \mathrm{d}\psi_j + (\mathcal{E} - \mathcal{V}_j)\psi_j * 1 = 0\,. \tag{A6}$$

It follows that for variations with support that include the junctions

$$\sum_j \int_{\partial M_j} (\mathcal{L}\bar{\psi}_j)(*\mathrm{d}\psi_j - W_j\psi_j\omega_j) = 0\,. \tag{A7}$$

We shall now assume that all extrema of interest are continuous at each junction and

$$\mathcal{L}\psi_j(J) = \mathcal{L}\psi(J) \qquad \forall J,\ j\,. \tag{A8}$$

hence the general junction condition is

$$\sum_j (*\mathrm{d}\psi_j - W_j\psi_j\omega_j) = 0\,. \tag{A9}$$

For the special case $\dim M = 1$, $\omega = 1$, $M_j = [L_J, L_j]$, $\partial M_j = L_j - L_J$, $\psi_j(J) = \psi(J)$ the junction conditions become

$$\sum_j \{(*\mathrm{d}\psi)_j - W_j\psi\}(J) = 0\,. \tag{A10}$$

Thus for each junction we demand

$$\sum_j ((*\mathrm{d}\psi)_j)(J) = \psi(J)\, W_J \tag{A11}$$

where $W_J = \sum_j W_j$ and the sum is over all branches that connect to junction node J. If we write

$$\mathrm{d}\psi_j = \psi_j' \mathrm{d}x^j \tag{A12}$$

(no j-sum implied), in terms of some coordinate x^j on branch j then $(*\mathrm{d}\psi)_j = \psi_j'$ and each condition may be written as

$$\sum_j \psi_j'(J) = W_J\psi(J)\,. \tag{A13}$$

Appendix B

In this appendix we present an alternative derivation of the properties of a point-like node by regarding the Schrödinger equation as the continuum limit of a tight-binding equation.

Let $\bigcup_{\mu=1}^{M}\{[0, L_\mu]_\mu\}$ denote the union of M copies of intervals of the real line and define $\mathcal{I}$ to be the space generated by identifying the 0 end of each $[0, L_\mu]_\mu$ $\forall\mu$. thus $\mathcal{I}$ is a one-dimensional M-star (having M arms) with a single junction. We are interested in writing down Schrödinger's equation on the space $\mathcal{C}(\mathcal{I})$ where $\mathcal{C} : \mathcal{I} \mapsto \mathbb{R}^3$ is a length preserving injective map into ordinary Euclidean space and deriving an appropriate junction condition. The approach is based on taking the continuum limit of a discrete quantum model based on tight-binding techniques.

To proceed let us first discretize $\mathcal{I}$ by adopting a mesh consisting of $d = \sum_{\mu=1}^{M}(N_\mu - 1) + 1$ points labelled $\{0, (1, \mu), (2, \mu), \ldots, (N_\mu, \mu)\}$ for each arm where 0 labels the common junction. We call this discretized space $\mathbb{I}$ and formulate a discrete linear field theory on $\mathbb{I}$ in terms of a d-dimensional vector space V with basis

$$\{|n, \mu\rangle, |0\rangle\} \tag{B1}$$

where $\mu \in \{1, \ldots, M\}$ and $n \in \{1, \ldots, N_\mu - 1\}$.

In the above basis, the Hamiltonian operator H possesses matrix elements of the form

$$\langle\mu, n|H|\mu, n\rangle = \epsilon \tag{B2}$$

$$\langle\mu, n_1|H|\mu, n_2\rangle = -\nu \qquad \text{if } n_1 = n_2 \pm 1,\ n_1, n_2 \in \{1, \ldots, N_\mu - 1\} \tag{B3}$$

$$\langle 0|H|0\rangle = \sigma \tag{B4}$$

$$\langle\mu, 1|H|0\rangle = -\omega \tag{B5}$$

$$\langle\mu_1, n_1|H|\mu_2, n_2\rangle = 0 \text{ otherwise.} \tag{B6}$$

For convenience, we have assumed that H is real and symmetric.

In the language of tight-binding descriptions, ϵ is the site energy excluding the junction, $-\nu$ the interaction energy of adjacent sites excluding the junction, σ is the site energy of the junction and $-\omega$ the interaction of the junction with its M neighbours.

The eigenvalues E of H are obtained by solving the coupled system

$$H|\psi\rangle = E|\psi\rangle \tag{B7}$$

i.e.

$$E\psi_{\mu,N_\mu-1} = \epsilon\psi_{\mu,N_\mu-1} - \nu\psi_{\mu,N_\mu-2} \tag{B8}$$

$$E\psi_{\mu,n} = \epsilon\psi_{\mu,n} - \nu(\psi_{\mu,n-1} + \psi_{\mu,n+1}) \qquad \text{where } n \in \{2, \ldots, N_\mu - 2\} \tag{B9}$$

$$E\psi_{\mu,1} = \epsilon\psi_{\mu,1} - \nu\psi_{\mu,2} - \omega\psi_0 \tag{B10}$$

$$E\psi_0 = \sigma\psi_0 - \omega\sum_{\mu=1}^{M}\psi_{\mu,1}\,. \tag{B11}$$

In terms of the natural metric on each arm let the common spacing between adjacent sites be a. We examine the continuum limit as $a \to 0$, $d \to \infty$ such that $aN_\mu = L_\mu$ is finite. To this end we introduce the map

$$\phi : \mathcal{I} \times \mathbb{R} \mapsto \mathbb{C}, \{x, a\} \mapsto \phi(x, a) \tag{B12}$$

and decompose it into ϕ^μ and $\hat{\phi}$, the restrictions to the μth arm and the junction of $\mathcal{I}$ respectively

$$\phi^\mu : \mathbb{R}^2 \mapsto \mathbb{C}, \{x, a\} \mapsto \phi(x, a) \tag{B13}$$

$$\hat{\phi} : \mathbb{R} \mapsto \mathbb{C}, \{a\} \mapsto \hat{\phi}(a) \tag{B14}$$

such that

$$\psi_n^\mu = \phi^\mu(an, a) \qquad \forall\mu \in \{1, \ldots, M\} \quad \forall n \in \{1, \ldots, N_\mu - 1\} \quad \forall a > 0 \tag{B15}$$

$$\psi_0 = \hat{\phi}(a) \qquad \forall a > 0\,. \tag{B16}$$

Thus equations (B8) to (B11) can be written

$$E(a)\phi^m(L_\mu - a, a) = \epsilon(a)\phi^m(L_\mu - a, a) - \nu(a)\phi^m(L_\mu - 2a, a) \tag{B17}$$

$$E(a)\phi^m(x, a) = \epsilon(a)\phi^m(x, a) - \nu(a)(\phi^m(x - a, a) + \phi^m(x + a, a))$$
$$\text{where } 2a \leqslant x \leqslant L_\mu - 2a \tag{B18}$$

$$E(a)\phi^m(a, a) = \epsilon(a)\phi^m(a, a) - \nu(a)\phi^m(2a, a) - \omega(a)\hat{\phi}(a) \tag{B19}$$

$$E(a)\hat{\phi}(a) = \sigma(a)\hat{\phi}(a) - \omega(a)\sum_{\mu=1}^{M}\phi^m(a, a). \tag{B20}$$

In order to get a well behaved limit of these equations we shall assume that the following Laurent expansions about $a = 0$ exist:

$$E(a) = E_0 + E_1 a + \cdots \tag{B21}$$

$$\epsilon(a) = \epsilon_{-2}a^{-2} + \epsilon_{-1}a^{-1} + \epsilon_0 a^0 + \epsilon_1 a^1 + \cdots \tag{B22}$$

$$\nu(a) = \nu_{-2}a^{-2} + \nu_{-1}a^{-1} + \nu_0 a^0 + \nu_1 a^1 + \cdots \tag{B23}$$

$$\omega(a) = \omega_{-2}a^{-2} + \omega_{-1}a^{-1} + \omega_0 a^0 + \omega_1 a^1 + \cdots \tag{B24}$$

$$\sigma(a) = \sigma_{-2}a^{-2} + \sigma_{-1}a^{-1} + \sigma_0 a^0 + \sigma_1 a^1 + \cdots . \tag{B25}$$

We proceed to expand ϕ^μ and $\hat{\phi}$ as a double Taylor series

$$\phi^\mu(x + b, a) = \phi^\mu(x, 0) + a\partial_a\phi^\mu(x, 0) + \frac{a^2}{2}\partial_a^2\phi^\mu(x, 0) + b\partial_x\phi^\mu(x, 0)$$
$$+ab\partial_x\partial_a\phi^\mu(x, 0) + \frac{b^2}{2}\partial_x^2\phi^\mu(x, 0)\cdots . \tag{B26}$$

For equations (B19) and (B20) involving $x = 0$, we note that since $\lim_{x\to 0^+}\phi^\mu(x, a) = \hat{\phi}(a)$ for all a, this series may be written

$$\phi^\mu(b, a) = \hat{\phi}(0) + a\partial_a\hat{\phi}(0) + \frac{a^2}{2}\partial_a^2\hat{\phi}(0) + b\partial_x\phi^\mu(0, 0) + ab\partial_x\partial_a\phi^\mu(0, 0)$$
$$+\frac{b^2}{2}\partial_x^2\phi^\mu(0, 0)\cdots \tag{B27}$$

$$\hat{\phi}(a) = \hat{\phi}(0) + a\partial_a\hat{\phi}(0) + \frac{a^2}{2}\partial_a^2\hat{\phi}(0) + \cdots \tag{B28}$$

where we assume that $\partial_x\phi^\mu(0, 0) = \lim_{x\to 0^+}(\partial_x\phi^\mu(x, 0))$ is well defined. Substituting these expansions into (B17), (B18), (B19) and (B20) we obtain the following series in a:

$$a^{-2}\phi^\mu(L_\mu, 0)(\nu_{-2} - \epsilon_{-2}) + a^{-1}\big[(\partial_a\phi^\mu(L_\mu, 0)(\nu_{-2} - \epsilon_{-2}) + \partial_x\phi^\mu(L_\mu, 0)(\epsilon_{-2} - 2\nu_{-2})$$
$$+\phi^\mu(L_\mu, 0)(\nu_{-1} - \epsilon_{-1})\big] + \bigg(\partial_a^2\phi^\mu(L_\mu, 0)\frac{(\nu_{-2} - \epsilon_{-2})}{2}$$
$$+\partial_a\partial_x\phi^\mu(L_\mu, 0)(\epsilon_{-2} - 2\nu_{-2}) + \partial_a\phi^\mu(L_\mu, 0)(\epsilon_{-1} - 2\nu_{-1})$$
$$+\partial_x^2\phi^\mu(L_\mu, 0)\frac{(4nu_{-2} - \epsilon_{-2})}{2} + \partial_x\phi^\mu(L_\mu, 0)(\epsilon_{-1} - 2\nu_{-1})$$
$$+\phi^\mu(L_\mu, 0)(E_0 + 2\nu_0 - \epsilon_0)\bigg)\cdots = 0 \tag{B29}$$

$$a^{-2}\phi^{\mu}(x,0)(2\nu_{-2}-\epsilon_{-2})+a^{-1}\big[(\partial_a\phi^{\mu}(x,0)(2\nu_{-2}-\epsilon_{-2})+\phi^{\mu}(x,0)(2\nu_{-1}-\epsilon_{-1})\big]$$
$$+\left(\frac{\partial_a^2\phi^{\mu}(x,0)(2\nu_{-2}-\epsilon_{-2})}{2}+\partial_a\phi^{\mu}(x,0)(2\nu_{-1}-\epsilon_{-1})\right.$$
$$\left.+\partial_x^2\phi^{\mu}(x,0)\nu_{-2}+\phi^{\mu}(x,0)(E_0+2\nu_0-\epsilon_0)\right)+\cdots=0 \tag{B30}$$

$$a^{-2}\hat{\phi}(0)(\nu_{-2}+\omega_{-2}-\epsilon_{-2})+a^{-1}\big[\partial_a\hat{\phi}(0)(\nu_{-2}+\omega_{-2}-\epsilon_{-2})+\partial_x\phi^{\mu}(0,0)(2\nu_{-2}-\epsilon_{-2})$$
$$+\hat{\phi}(0)(\nu_{-1}+\omega_{-1}-\epsilon_{-1})\big]+\left(\frac{\partial_a^2\hat{\phi}(0)(\nu_{-2}+\omega_{-2}-\epsilon_{-2})}{2}\right.$$
$$+\partial_a\partial_x\phi^{\mu}(0,0)(2\nu_{-2}-\epsilon_{-2})+\partial_a\hat{\phi}(0)(\nu_{-1}+\omega_{-1}-\epsilon_{-1})$$
$$+\partial_x^2\phi^{\mu}(0,0)\frac{(4\nu_{-2}-\epsilon_{-2})}{2}+\partial_x\phi^{\mu}(0,0)(2\nu_{-1}-\epsilon_{-1})$$
$$\left.+\hat{\phi}(0)\big[E_0+(\nu_0+\omega_0-\epsilon_0)\big]\right)+\cdots=0 \tag{B31}$$

$$a^{-2}\hat{\phi}(0)(M\omega_{-2}-\sigma_{-2})+a^{-1}\left(\partial_a\hat{\phi}(0)(M\omega_{-2}-\sigma_{-2})+\hat{\phi}(0)(M\omega_{-1}-\sigma_{-1})\right.$$
$$\left.+\omega_{-2}\sum_{\mu=1}^{M}\partial_x\phi^{\mu}(0,0)\right)+\left(\frac{\partial_a^2\hat{\phi}(0)(M\omega_{-2}-\sigma_{-2})}{2}+\partial_a\hat{\phi}(0)(M\omega_{-1}-\sigma_{-1})\right.$$
$$+\hat{\phi}(0)(E_0+M\omega_0-\sigma_0)+\omega_{-2}\sum_{\mu=1}^{M}\partial_a\partial_x\phi^{\mu}(0,0)+\frac{\omega_{-2}}{2}\sum_{\mu=1}^{M}\partial_x^2\phi^{\mu}(0,0)$$
$$\left.+\omega_{-1}\sum_{\mu=1}^{M}\partial_x\phi^{\mu}(0,0)\right)+\cdots=0\,. \tag{B32}$$

From (B30) we see that the term in a^{-2} will vanish if $2\nu_{-2}=\epsilon_{-2}$ and the term in a^{-1} will vanish if $2\nu_{-1}=\epsilon_{-1}$. Thus we recover Schrödinger's equation with $2\nu_0=\epsilon_0$ and $\nu_{-2}=\frac{\hbar^2}{2m}$.

$$\frac{-\hbar^2}{2m}\partial_x^2\phi^{\mu}(x,0)=E_0\phi^{\mu}(x,0)\,. \tag{B33}$$

The higher-order terms can be made to vanish for appropriate choices of higher-order derivatives in the expansions. From (B29) we see that the term in a^{-2} will vanish if

$$\phi^{\mu}(L_\mu,0)=0 \tag{B34}$$

which we recognize as a standard boundary condition. From (B31) we see that the term in a^{-2} will vanish if $\omega_{-2}=\nu_{-2}$, and the term in a^{-1} will vanish if $\omega_{-1}=\nu_{-1}$. Thus Schrödinger's equation extends to the junction if $\omega_0=\nu_0$

$$\frac{-\hbar^2}{2m}\partial_x^2\phi^{\mu}(0,0)=E_0\hat{\phi}(0). \tag{B35}$$

From (B32) we see that the term in a^{-2} will vanish if $M\omega_{-2} = \sigma_{-2}$. The term in a^{-1} now gives us the boundary condition for the junction. If we write $2m(M\omega_{-1} - \sigma_{-1})/\hbar^2 \equiv W$ then we require

$$W\hat{\phi}(0) + \sum_{\mu=1}^{M} \partial_x \phi^\mu(0,0) = 0 . \tag{B36}$$

The higher-order terms can be made to vanish for appropriate choices of higher-order derivatives in the expansion. Equation (B33) together with the boundary conditions (B34) and (B36) are sufficient to determine the eigenvalues E in terms of W and the lengths $\{L_\mu\}$.

References

[1] Avishai Y and Luck J M 1992 *Phys. Rev.* B **45** 1074
[2] Exner P and Šeba P 1987 *Phys. Lett.* **128A** 493
[3] Exner P and Šeba P 1989 *Rep. Math. Phys.* **28** 7
[4] Avishai Y, Hatsugai Y and Kohmoto M 1993 *Phys. Rev.* B **47** 9561
[5] Doucot B and Rammal R 1986 *J. Physique* **47** 973
[6] Ruedenberg K and Scherr C W 1953 *J. Chem. Phys* **21** 1565
[7] Avron J E, Raveh A and Zur B 1988 *Rev. Mod. Phys.* **60** 873
[8] Shapiro B 1983 *Phys. Rev. Lett.* **50** 747
[9] Buttiker M 1985 *Phys. Rev.* B **32** 1985
[10] Cahay M, Bandyopadhyay S and Grubin H L 1989 *Phys. Rev.* B **39** 12989
[11] Kowel D, Sivan U, Entin-Wohlman O and Imry Y 1990 *Phys. Rev.* B **42** 9009
[12] Benn I M and Tucker R W 1989 *Phys. Rev.* D **39** 1594
[13] Robinson S J and Jeffery M 1994 Conductance fluctuations in multiply connected normal wire networks *Preprint* (submitted to *Phys. Rev.* B)