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Dirichlet-to-Neumann Mapping for the Characteristic Elliptic Equations with Symmetric Periodic Coefficients

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Abstract. Based on the numerical evidences, an analytical expression of the Dirichlet-to-Neumann mapping in the form of infinite product was first conjectured for the one-dimensional characteristic Schrödinger equation with a sinusoidal potential in [Commun. Comput. Phys., 3(3): 641-658, 2008]. It was later extended for the general second-order characteristic elliptic equations with symmetric periodic coefficients in [J. Comp. Phys., 227: 6877-6894, 2008]. In this paper, we present a proof for this Dirichlet-to-Neumann mapping.

AMS subject classifications: 65M99, 81-08

Key words: Dirichlet-to-Neumann mapping, Schrödinger equation, symmetric periodic potentials, absorbing boundary conditions.

1 Introduction

Periodic structure problems largely exist in the science and engineering such as semiconductor nanostructures, semiconductor superlattices [3,24], photonic crystals (PC) structures [2,15,18], meta materials [20] and Bragg gratings of surface plasmon polariton (SPP) waveguides [11,19]. Usually they are modeled by partial differential equations with periodic coefficients and/or periodic geometries. In order to numerically solve these equations efficiently, one usually confines the computational domain by introducing artificial boundaries and imposing suitable boundary conditions on them. For wave-like equations, the ideal boundary conditions should not only lead to well–posed problems, but also mimic the perfect absorption of waves which travel out of the computational domain

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through the artificial boundaries. Right in this sense, these boundary conditions are usually called absorbing (or transparent, non-reflecting in the same spirit) in the literature.

The study of absorbing boundary conditions (ABCs) for linear wave-like equations has been a hot research topic for many years and significant developments have been made on their designing and implementing. The interested reader is referred to the review papers [1, 8, 10, 23]. Comparatively, the study of exact or approximate ABCs for periodic structure problems is relatively a very current research topic, cf. the recent papers [6,7,14,21,22,25,26]. For a review on the theory and numerical techniques of waves in locally periodic media we refer the reader to [4,9,12].

Based on the numerical evidences, one of the authors [28] conjectured an exact ABC in the form of Dirichlet-to-Neumann (DtN) mapping for the characteristic Schrödinger equation

$$\left[-\partial_x^2+V(x)\right]y=zy, \tag{1.1}$$

when the potential V is sinusoidal. This DtN mapping is expressed as an infinite product

$$\frac{y'(0)}{y(0)}=-\sqrt{-z+\mu_{0,V}^{NN}}\prod_{m=1}^{+\infty}\frac{\sqrt{-z+\mu_{m,V}^{NN}}}{\sqrt{-z+\mu_{m,V}^{DD}}},\quad \Im z>0, \tag{1.2}$$

where $\{\mu_{r,V}^{NN}\}_{r\geq 0}$ are eigenvalues of the Schrödinger operator $-\partial_x^2+V(x)$ with Neumann boundary conditions imposed on the periodic cell boundaries, and $\{\mu_{r,V}^{DD}\}_{r\geq 1}$ are eigenvalues with Dirichlet boundary conditions imposed. This DtN mapping was then extended in [5] for the general second-order characteristic elliptic equations

$$\left[-\partial_x m^{-1}(x)\partial_x+V(x)\right]y=\rho(x)zy,\quad \forall x\geq 0, \tag{1.3}$$

where ρ, V and m are supposed to be symmetric periodic. The exact DtN mapping for (1.3) was conjectured to be

$$\frac{y'(0)}{y(0)}=-\sqrt{c(0)\rho(0)}\sqrt{-z+\mu_{0,V}^{NN}}\prod_{m=1}^{+\infty}\frac{\sqrt{-z+\mu_{m,V}^{NN}}}{\sqrt{-z+\mu_{m,V}^{DD}}},\quad \Im z>0, \tag{1.4}$$

where again, $\{\mu_{r,V}^{NN}\}_{r\geq 0}$ are the eigenvalues of characteristic elliptic equations (1.3) with Neumann boundary conditions and $\{\mu_{r,V}^{DD}\}_{r\geq 1}$ with Dirichlet boundary conditions specified on the periodic cell boundaries. The exact DtN mapping (1.4) was used in [5] to design the exact ABCs for a set of one-dimensional time-dependent wave equations with symmetric periodic coefficients.

In this paper, we give a proof for the DtN mapping expression (1.4). Our idea was stimulated by the work of J. Pöschel and E. Trubowitz. In [17], they considered the characteristic Schrödinger equation (1.1) with 1-periodic potentials. For the basic solution φ

satisfying the initial conditions $y(0)=0$, $y'(0)=1$, they derived an analytic expression of φ evaluating at $x=1$ as

$$\varphi(1;z)=\prod_{m\geq 1}\frac{\mu_{m,V}^{DD}-z}{m^2\pi^2}, \tag{1.5}$$

where $\{\mu_{m,V}^{DD}\}_{m\geq 1}$ are the eigenvalues of (1.1) with Dirichlet boundary conditions imposed on both ends of a single periodic cell. Mimicking their deducing, we give analytical expressions of an infinite product for all basic solutions of (1.1) and their spatial derivatives at the origin. The DtN mapping (1.2) is then derived after investigating the relations of eigenvalues associated with different boundary conditions under the assumption that the potential V is symmetric.

The organization of the rest is as follows. In Section 2, we introduce a transformation matrix T_c of (1.1) within a single 1-periodic cell. It turns out that any element of T_c admits an expression in a form analogous to (1.5). Based on this expression of T_c, we present our main result and give an exact expression of DtN mapping in Section 3. The more general characteristic elliptic equations will be considered in Section 4, and the DtN mapping (1.4) is derived by a simple scaling argument.

2 Analytic expression for cell transformation matrix

The characteristic Schrödinger equation (1.1) can be transformed into a first order ODE system

$$\frac{\mathrm{d}}{\mathrm{dx}}\begin{bmatrix} y \\ y' \end{bmatrix}=\begin{bmatrix} 0 & 1 \\ V(x)-z & 0 \end{bmatrix}\begin{bmatrix} y \\ y' \end{bmatrix}. \tag{2.1}$$

Given two points x_1 and x_2, the ODE system (2.1) determines a transformation matrix $T(x_2,x_1;z)$ on $\mathbb{R}^2$, for any solution y of (1.1) which satisfies

$$\begin{bmatrix} y(x_2) \\ y'(x_2) \end{bmatrix}=T(x_2,x_1;z)\begin{bmatrix} y(x_1) \\ y'(x_1) \end{bmatrix}. \tag{2.2}$$

Obviously, T admits the following properties

$$T(x,x;z)=I_{2\times 2},\quad T(x_3,x_2;z)T(x_2,x_1;z)=T(x_3,x_1;z), \tag{2.3a}$$

$$\det T(x_2,x_1;z)=1,\quad T(x_2+1,x_1+1;z)=T(x_2,x_1;z). \tag{2.3b}$$

Let $\theta=\theta(x;z)$ be the solution of (1.1) with initial conditions $y(0)=1$ and $y'(0)=0$, and $\varphi=\varphi(x;z)$ with initial conditions $y(0)=0$ and $y'(0)=1$, the cell transformation matrix $T_c(z)=T(1,0;z)$ is then given by

$$T_c(z)=\begin{bmatrix} \theta(1;z) & \varphi(1;z) \\ \theta'(1;z) & \varphi'(1;z) \end{bmatrix}\triangleq\begin{bmatrix} t_{ND}(z) & t_{DD}(z) \\ t_{NN}(z) & t_{DN}(z) \end{bmatrix}, \tag{2.4}$$

where we have denoted the elements of T_c by $t_{\alpha\beta}$ with $\alpha,\beta\in\{D,N\}$. In the rest of this section, we intend to present analytical expressions for $t_{\alpha\beta}$.

If $V(x)\equiv 0$, it is known that

$$\theta(x;z)=\cos(\sqrt{z}x),\quad \varphi(x;z)=\frac{\sin(\sqrt{z}x)}{\sqrt{z}}.$$

Since

$$\cos\sqrt{z}=\prod_{m\geq 1}\frac{\frac{(2m-1)^2\pi^2}{4}-z}{\frac{(2m-1)^2\pi^2}{4}},\quad \frac{\sin\sqrt{z}}{\sqrt{z}}=\prod_{m\geq 1}\frac{m^2\pi^2-z}{m^2\pi^2},$$

the elements of T_c can be expressed into the form of infinite products, i.e.,

$$t_{ND}(z)=\prod_{m\geq 1}\frac{\frac{(2m-1)^2\pi^2}{4}-z}{\frac{(2m-1)^2\pi^2}{4}},\quad t_{DD}(z)=\prod_{m\geq 1}\frac{m^2\pi^2-z}{m^2\pi^2},\tag{2.5a}$$

$$t_{NN}(z)=-z\prod_{m\geq 1}\frac{m^2\pi^2-z}{m^2\pi^2},\quad t_{DN}(z)=\prod_{m\geq 1}\frac{\frac{(2m-1)^2\pi^2}{4}-z}{\frac{(2m-1)^2\pi^2}{4}}.\tag{2.5b}$$

For the brevity of notations, we introduce

$$\mu^{DD}_{m,0}=\mu^{NN}_{m,0}=m^2\pi^2,\qquad \mu^{ND}_{m,0}=\mu^{DN}_{m,0}=\frac{(2m-1)^2\pi^2}{4},$$

where D and N stand for *Dirichlet* and *Neumann* respectively. It is easy to verify that for $m\geq 1$, $\mu^{DD}_{m,0}$, $\mu^{DN}_{m,0}$ and $\mu^{ND}_{m,0}$ are the eigenvalues of (1.1) equipped with the corresponding boundary conditions on the reference periodic cell $[0,1]$, and this is also the case for $\mu^{NN}_{m,0}$ with $m\geq 0$. Therefore, we can rewrite (2.5) into the following more inspiring form

$$t_{ND}(z)=\prod_{m\geq 1}\frac{\mu^{ND}_{m,0}-z}{\mu^{ND}_{m,0}},\quad t_{DD}(z)=\prod_{m\geq 1}\frac{\mu^{DD}_{m,0}-z}{\mu^{DD}_{m,0}},\tag{2.6a}$$

$$t_{NN}(z)=(\mu^{NN}_{0,0}-z)\prod_{m\geq 1}\frac{\mu^{NN}_{m,0}-z}{\mu^{NN}_{m,0}},\quad t_{DN}(z)=\prod_{m\geq 1}\frac{\mu^{DN}_{m,0}-z}{\mu^{DN}_{m,0}}.\tag{2.6b}$$

For a general periodic potential V, Pöschel and Trubowitz [17] presented an analytical expression of $\varphi(1;z)$, the (1,2)-element of T_c, as

$$t_{DD}(z)=\prod_{m\geq 1}\frac{\mu^{DD}_{m,V}-z}{\mu^{DD}_{m,0}},\tag{2.7}$$

where $\mu^{DD}_{m,V}$ with $m\geq 1$ are the eigenvalues of (1.1) with Dirichlet boundary conditions imposed on the cell boundary. Actually, for the other three elements of T_c, we have analogous results.

Theorem 2.1. *Given a general smooth 1-periodic potential $V(x)$, we have*

$$t_{ND}(z)=\prod_{m\geq 1}\frac{\mu_{m,V}^{ND}-z}{\mu_{m,0}^{ND}},\quad t_{DD}(z)=\prod_{m\geq 1}\frac{\mu_{m,V}^{DD}-z}{\mu_{m,0}^{DD}}, \tag{2.8a}$$

$$t_{NN}(z)=(\mu_{0,V}^{NN}-z)\prod_{m\geq 1}\frac{\mu_{m,V}^{NN}-z}{\mu_{m,0}^{NN}},\quad t_{DN}(z)=\prod_{m\geq 1}\frac{\mu_{m,V}^{DN}-z}{\mu_{m,0}^{DN}}, \tag{2.8b}$$

where $\{\mu_{m,V}^{ND},\mu_{m,V}^{DD},\mu_{m,V}^{NN},\mu_{m,V}^{DN}\}$ are the eigenvalues of (1.1) *with boundary conditions*

$$\begin{aligned} &ND: y'(0)=y(1)=0, && DD: y(0)=y(1)=0,\\ &NN: y'(0)=y'(1)=0, && DN: y(0)=y'(1)=0. \end{aligned}$$

To prove the above, we mimic the reasoning in [17] for the derivation of (2.7).

Lemma 2.1. *For any $\alpha,\beta\in\{D,N\}$, it holds that*

$$\mu_{m,0}^{\alpha\beta}-\|V\|_\infty\leq\mu_{m,V}^{\alpha\beta}\leq\mu_{m,0}^{\alpha\beta}+\|V\|_\infty.$$

Proof. Let us introduce

$$\begin{aligned} &H_{DD}=H_0^1(0,1), && H_{DN}=\{f\in H^1(0,1): f(0)=0\},\\ &H_{NN}=H^1(0,1), && H_{ND}=\{f\in H^1(0,1): f(1)=0\}, \end{aligned}$$

and

$$a_V(\varphi,k)=\int_0^1[\varphi'(x)k'(x)+V(x)\varphi(x)k(x)]dx,\quad a_0(\varphi,k)=\int_0^1\varphi'(x)k'(x)dx.$$

The weak form of the characteristic equation (1.1) is to find $\mu\in\mathbb{R}$ and $0\neq\varphi\in H_{\alpha\beta}$, such that

$$a_V(\varphi,k)=\mu(\varphi,k),\quad \forall k\in H_{\alpha\beta}.$$

Thanks to the min-max expression for eigenvalues, we have

$$\mu_{m,V}^{\alpha\beta}=\min_{D\subset H_{\alpha\beta}}\max_{y\in D}\frac{a_V(y,y)}{(y,y)},$$

where $\dim D=m$ with $m\geq 1$ for H_{DD}, H_{DN} and H_{ND}, and $\dim D=m+1$ with $m\geq 0$ for H_{NN}. Since

$$a_0(\varphi,\varphi)-||V||_\infty(\varphi,\varphi)\leq a_V(\varphi,\varphi)\leq a_0(\varphi,\varphi)+||V||_\infty(\varphi,\varphi),$$

we have

$$\mu_{m,0}^{\alpha\beta}-\|V\|_\infty\leq\mu_{m,V}^{\alpha\beta}\leq\mu_{m,0}^{\alpha\beta}+\|V\|_\infty.$$

The proof thus finishes. $\square$

Lemma 2.2. *There exists a constant $C>0$, such that for any $z\in\mathbb{C}$ with $|z-(m-1/2)\pi|\geq\pi/4$ for any integer m, it holds that*

$$\exp|\Im z|\leq C|\cos z|,$$

and for any z with $|z-m\pi|\geq\pi/4$ for any integer m, it holds that

$$\exp|\Im z|\leq C|\sin z|.$$

Proof. Write $z=x+iy$ with real x and y. Let us introduce

$$P(z)=\frac{\exp(2|\Im z|)}{|\cos z|^2},\qquad Q(z)=\frac{\exp(2|\Im z|)}{|\sin z|^2}.$$

Since

$$P(z)=\frac{\exp(2|y|)}{\cosh^2 y-\sin^2 x},\qquad Q(z)=\frac{\exp(2|y|)}{\cosh^2 y-\cos^2 x},$$

we have

$$\lim_{y\to\infty}P(z)=\lim_{y\to\infty}Q(z)=4.$$

The proof finishes by considering that both P and Q are π-periodic in the x-direction. $\square$

Lemma 2.3. *For any $\alpha,\beta\in\{D,N\}$, the infinite products*

$$f_{ND;V}(z)=\prod_{m\geq 1}\frac{\mu_{m,V}^{ND}-z}{\mu_{m,0}^{ND}},\quad f_{DD;V}(z)=\prod_{m\geq 1}\frac{\mu_{m,V}^{DD}-z}{\mu_{m,0}^{DD}},$$
$$f_{NN;V}(z)=(\mu_{0,V}^{NN}-z)\prod_{m\geq 1}\frac{\mu_{m,V}^{NN}-z}{\mu_{m,0}^{NN}},\quad f_{DN;V}(z)=\prod_{m\geq 1}\frac{\mu_{m,V}^{DN}-z}{\mu_{m,0}^{DN}}$$

are entire functions of z, whose roots are precisely $\mu_{m,V}^{\alpha\beta}$. Besides, we have

$$f_{ND;0}(z)=f_{DN;0}(z)=\cos\sqrt{z},\quad f_{DD;0}(z)=\frac{\sin\sqrt{z}}{\sqrt{z}},\quad f_{NN;0}(z)=-\sqrt{z}\sin\sqrt{z}.$$

Furthermore, the following

$$f_{\alpha\beta;V}(z)=f_{\alpha\beta;0}(z)\left[1+\mathcal{O}\left(\frac{\log n}{n}\right)\right]$$

holds uniformly on the circles $|z|=(n+\delta_{\alpha,\beta}/2)^2\pi^2$. Here δ denotes the Kronecker symbol.

Proof. By Lemma 2.1, $\mu_{m,V}^{\alpha\beta}-\mu_{m,0}^{\alpha\beta}$ is uniformly bounded with respect to m. Since $\mu_{m,0}^{\alpha\beta}=\mathcal{O}(m^{-2})$, this implies that

$$\sum_{m\geq 1}\left|\frac{\mu_{m,V}^{\alpha\beta}-z}{\mu_{m,0}^{\alpha\beta}}-1\right|=\sum_{m\geq 1}\left|\frac{\mu_{m,V}^{\alpha\beta}-\mu_{m,0}^{\alpha\beta}-z}{\mu_{m,0}^{\alpha\beta}}\right|$$

converges uniformly on any bounded subset of $\mathbb{C}$. Therefore, the infinite product $f_{\alpha\beta;V}$ converges to an entire function of z, whose roots are precisely $\mu_{m,V}^{\alpha\beta}$. On the circle $|z|=(n+\delta_{\alpha,\beta}/2)^2\pi^2$, we have

$$a_m^{\alpha\beta}(z)\triangleq\frac{\mu_{m,V}^{\alpha\beta}-z}{\mu_{m,0}^{\alpha\beta}-z}-1=\begin{cases}\mathcal{O}(\frac{1}{n}), & m=n,\\ \mathcal{O}\big(\frac{1}{|m^2-n^2|}\big), & m\neq n.\end{cases}\tag{2.9}$$

Since

$$\begin{aligned}\sum_{m\geq 1,m\neq n}\frac{1}{|m^2-n^2|}&=\sum_{1\leq m\leq 2n,m\neq n}\frac{1}{|m-n|}\frac{1}{m+n}+\sum_{m>2n}\frac{1}{|m^2-n^2|}\\&\leq\frac{2}{n}\sum_{1\leq k\leq n}\frac{1}{k}+\sum_{k>n}\frac{1}{k^2}\leq\frac{2}{n}(1+\log n)+\frac{1}{n}=\mathcal{O}\left(\frac{\log n}{n}\right),\end{aligned}\tag{2.10}$$

we derive

$$\begin{aligned}\left|\prod_{m\geq 1,m\neq n}[1+a_m^{\alpha\beta}(z)]-1\right|&\leq\prod_{m\geq 1,m\neq n}[1+|a_m^{\alpha\beta}(z)|]-1\leq\exp\sum_{m\geq 1,m\neq n}|a_m^{\alpha\beta}(z)|-1\\&\leq\exp\left[\mathcal{O}\left(\frac{\log n}{n}\right)\right]-1=\mathcal{O}\left(\frac{\log n}{n}\right).\end{aligned}\tag{2.11}$$

This implies that the following

$$\prod_{m\geq 1}\frac{\mu_{m,V}^{\alpha\beta}-z}{\mu_{m,0}^{\alpha\beta}-z}=\left[1+\mathcal{O}\left(\frac{1}{n}\right)\right]\left[1+\mathcal{O}\left(\frac{\log n}{n}\right)\right]=1+\mathcal{O}\left(\frac{\log n}{n}\right)$$

holds uniformly on the circles $|z|=(n+\delta_{\alpha,\beta}/2)^2\pi^2$. The proof thus finishes by recalling (2.5). $\square$

Proof of Theorem 2.1. We first recall the basic estimates of the elements of T_c given in [17]:

$$\begin{aligned}&\left|t_{ND}(z)-\cos\sqrt{z}\right|\leq\frac{1}{|\sqrt{z}|}\exp\left(|\Im\sqrt{z}|+\|V\|_2\right),\\&\left|t_{DD}(z)-\frac{\sin\sqrt{z}}{\sqrt{z}}\right|\leq\frac{1}{|z|}\exp\left(|\Im\sqrt{z}|+\|V\|_2\right),\\&\left|t_{NN}(z)+\sqrt{z}\sin\sqrt{z}\right|\leq\|V\|_2\exp\left(|\Im\sqrt{z}|+\|V\|_2\right),\\&\left|t_{DN}(z)-\cos\sqrt{z}\right|\leq\frac{\|V\|_2}{|\sqrt{z}|}\exp\left(|\Im\sqrt{z}|+\|V\|_2\right).\end{aligned}$$

The above implies that

$$\begin{aligned}&t_{ND}(z)=\cos\sqrt{z}+\mathcal{O}\left(\frac{\exp|\Im\sqrt{z}|}{|\sqrt{z}|}\right),\quad t_{DD}(z)=\frac{\sin\sqrt{z}}{\sqrt{z}}+\mathcal{O}\left(\frac{\exp(\Im\sqrt{z})}{|z|}\right),\\&t_{NN}(z)=-\sqrt{z}\sin\sqrt{z}+\mathcal{O}\left(\exp|\Im\sqrt{z}|\right),\quad t_{DN}(z)=\cos\sqrt{z}+\mathcal{O}\left(\frac{\exp|\Im\sqrt{z}|}{|\sqrt{z}|}\right).\end{aligned}$$

Using Lemma 2.2, on the circles $|z|=(n+\delta_{\alpha,\beta}/2)^2\pi^2$ for n large enough, we have

$$t_{ND}(z)=\cos\sqrt{z}\left[1+\mathcal{O}\left(\frac{1}{n}\right)\right],\quad t_{DD}(z)=\frac{\sin\sqrt{z}}{\sqrt{z}}\left[1+\mathcal{O}\left(\frac{1}{n}\right)\right],$$
$$t_{NN}(z)=-\sqrt{z}\sin\sqrt{z}\left[1+\mathcal{O}\left(\frac{1}{n}\right)\right],\quad t_{DN}(z)=\cos\sqrt{z}\left[1+\mathcal{O}\left(\frac{1}{n}\right)\right].$$

Applying Lemma 2.3, we derive

$$t_{\alpha\beta}(z)=f_{\alpha\beta;V}(z)\left[1+\mathcal{O}\left(\frac{\log n}{n}\right)\right],\quad \forall\alpha,\beta\in\{D,N\}. \tag{2.12}$$

Both $t_{\alpha\beta}$ and $f_{\alpha\beta;V}$ are entire functions of z. Since $f_{\alpha\beta;V}$ have same zeroes as $t_{\alpha\beta}$, their quotients are also entire. The estimate (2.12) implies that

$$\lim_{n\to+\infty}\sup_{|z|=(n+\delta_{\alpha,\beta}/2)^2\pi^2}\left|\frac{t_{\alpha\beta}(z)}{f_{\alpha\beta;V}(z)}-1\right|=0.$$

The proof of Theorem 2.1 thus ends by Liouville's theorem. □

3 Analytical expression of the Dirichlet-to-Neumann map

According to (2.3), the cell transformation matrix $T_c(z)=T(1,0;z)$ has two eigenvalues σ and $1/\sigma$ with $0<|\sigma|\le 1$. If $\Im z\neq 0$, we have $|\sigma|<1$. The associated eigenvectors, denoted by $(c_+,d_+)^\top$ and $(c_-,d_-)^\top$, are thus linearly independent. Therefore, $T(x,0;z)(c_\pm,d_\pm)^\top$ are two linearly independent solutions of the ODE system (2.1). By setting $\mu=\ln\sigma$, it is straightforward to verify that

$$\begin{aligned}e^{\pm\mu(1+x)}T(1+x,0;z)(c_\mp,d_\mp)^\top &=e^{\pm\mu x}e^{\pm\mu}T(1+x,1;z)T_c(z)(c_\mp,d_\mp)^\top\\ &=\sigma^{\mp 1}e^{\pm\mu x}e^{\pm\mu}T(x,0;z)(c_\mp,d_\mp)^\top\\ &=e^{\pm\mu x}T(x,0;z)(c_\mp,d_\mp)^\top.\end{aligned}$$

This implies that $e^{\pm\mu x}T(x,0;z)(c_\mp,d_\mp)^\top$ are 1-periodic functions. Since $\Re\mu<0$, we conclude that

$$T(x,0;z)(c_+,d_+)^\top=e^{\mu x}e^{-\mu x}T(x,0;z)(c_+,d_+)^\top$$

is bounded in $\mathbb{R}^+$, while

$$T(x,0;z)(c_-,d_-)^\top=e^{-\mu x}e^{\mu x}T(x,0;z)(c_-,d_-)^\top$$

is unbounded in $\mathbb{R}^+$. Since

$$\sigma c_+=c_+\theta(1;z)+d_+\varphi(1;z),$$

the DtN mapping $I(z)$, defined as the quotient of the Neumann data over the Dirichlet data at $x=0$ for the bounded solution in $\mathbb{R}^+$, is then given by

$$I(z)=\frac{d_+}{c_+}=-\frac{\theta(1;z)-\sigma}{\varphi(1;z)}=-\frac{t_{ND}(z)-\sigma}{t_{DD}(z)}. \tag{3.1}$$

On the other hand, the characteristic equation of the cell transformation matrix T_c is

$$\sigma^2-\Delta(z)\sigma+1=0, \tag{3.2}$$

where we have set $\Delta(z)=t_{ND}(z)+t_{DN}(z)$. For any z with $\Im z\neq 0$, the root of (3.2) with smaller modulus is

$$\sigma=\left(1-\sqrt{\frac{\Delta(z)-2}{\Delta(z)+2}}\right)\Big/\left(1+\sqrt{\frac{\Delta(z)-2}{\Delta(z)+2}}\right). \tag{3.3}$$

In the above, $\sqrt{\cdot}$ denotes the square root function with $\sqrt{1}=1$. The branch cut is set as the negative real axis. Formally, Δ and σ can be computed with (3.3) by using the expression (2.8). But there exist more elegant formulations. Actually, considering asymptotically $t_{ND}(z)\sim\cos(\sqrt{z})$ and $t_{DN}(z)\sim\cos(\sqrt{z})$, we have

$$\Delta(z)-2=t_{ND}(z)+t_{DN}(z)-2\sim 2\cos(\sqrt{z})-2=-4\sin^2\frac{\sqrt{z}}{2},$$

and

$$\Delta(z)+2=t_{ND}(z)+t_{DN}(z)+2\sim 2\cos(\sqrt{z})+2=4\cos^2\frac{\sqrt{z}}{2}.$$

Following the same reasonings for deriving (2.8), we have

$$\Delta(z)-2=(\mu_0-z)\prod_{m\geq 1}\frac{(\mu_{2m-1}-z)(\mu_{2m}-z)}{\mu^{NN}_{2m,0}\mu^{DD}_{2m,0}}, \tag{3.4a}$$

$$\Delta(z)+2=4\prod_{m\geq 1}\frac{(\mu'_{2m-1}-z)(\mu'_{2m}-z)}{\mu^{NN}_{2m-1,0}\mu^{DD}_{2m-1,0}}, \tag{3.4b}$$

where $\{\mu_m\}$ are the roots of equation $\Delta(z)-2=0$, and $\{\mu'_m\}$ are the roots of equation $\Delta(z)+2=0$. According to Theorem 2.1 in [16], $\{\mu_m\}$ and $\{\mu'_m\}$ can be ordered as

$$\mu_0<\mu'_1\leq\mu'_2<\mu_1\leq\mu_2<\mu'_3\leq\mu'_4<\mu_3\leq\mu_4<\cdots.$$

Besides, μ_m coincide with the eigenvalues of periodic boundary problem

$$\begin{cases}-y''+V(x)y=zy,\\ y(0)=y(1),\quad y'(0)=y'(1),\end{cases} \tag{3.5}$$

and μ'_m coincide with the eigenvalues of anti-periodic boundary problem

$$\begin{cases}-y''+V(x)y=zy,\\ y(0)+y(1)=0,\quad y'(0)+y'(1)=0.\end{cases} \tag{3.6}$$

Theorem 3.1. *If the periodic potential $V(x)$ is symmetric, i.e., $V(-x)=V(x)$, we have*

$$\mu_{0,V}^{NN}=\mu_0,\ \ \{\mu_{2m-1,V}^{NN},\mu_{2m-1,V}^{DD}\}=\{\mu'_{2m-1},\mu'_{2m}\},\ \ \{\mu_{2m,V}^{NN},\mu_{2m,V}^{DD}\}=\{\mu_{2m-1},\mu_{2m}\},\ \ \forall m\geq 1.$$

Proof. If V is symmetric, then θ is even and φ is odd. Let us put

$$A(z)=T\left(1,\frac{1}{2};z\right),\quad B(z)=T\left(\frac{1}{2},0;z\right).$$

Then we have

$$A^{-1}(z)=T\left(\frac{1}{2},1;z\right)=T\left(-\frac{1}{2},0;z\right)=\begin{bmatrix}\theta(-\frac{1}{2},z) & \varphi(-\frac{1}{2},z)\\ \theta'(-\frac{1}{2},z) & \varphi'(-\frac{1}{2},z)\end{bmatrix}=\begin{bmatrix}\theta(\frac{1}{2},z) & -\varphi(\frac{1}{2},z)\\ -\theta'(\frac{1}{2},z) & \varphi'(\frac{1}{2},z)\end{bmatrix}.$$

A direct computation shows that

$$\begin{aligned}T_c(z)-I&=A(z)B(z)-I=A(z)[B(z)-A^{-1}(z)]=A(z)\begin{bmatrix}0 & 2\varphi(\frac{1}{2},z)\\ 2\theta'(\frac{1}{2},z) & 0\end{bmatrix},\\ T_c(z)+I&=A(z)B(z)+I=A(z)[B(z)+A^{-1}(z)]=A(z)\begin{bmatrix}2\theta(\frac{1}{2},z) & 0\\ 0 & 2\varphi'(\frac{1}{2},z)\end{bmatrix}.\end{aligned}$$

If λ is an eigenvalue of periodic boundary problem (3.5), then $\det(T_c(\lambda)-I)=0$, and we have either $\varphi(1/2,\lambda)=0$ or $\theta'(1/2,\lambda)=0$. The former implies that $\varphi(0,\lambda)=\varphi(1,\lambda)=0$ and thus $(\lambda,\varphi(\cdot,\lambda))$ is an eigenpair of Dirichlet boundary problem. The latter implies that $\theta'(0,\lambda)=\theta'(1,\lambda)=0$ and thus $(\lambda,\theta(\cdot,\lambda))$ is an eigenpair of Neumann boundary problem. Analogously, if λ is an eigenvalue of anti-periodic boundary problem (3.6), then $\det(T_c(\lambda)+I)=0$, and we have either $\theta(1/2,\lambda)=0$ or $\varphi'(1/2,\lambda)=0$. The former implies that $\theta'(0,\lambda)=\theta'(1,\lambda)=0$ and thus $(\lambda,\theta(\cdot,\lambda))$ is an eigenpair of Neumann boundary problem. The latter implies that $\varphi(0,\lambda)=\varphi(1,\lambda)=0$ and thus $(\lambda,\varphi(\cdot,\lambda))$ is an eigenpair of Dirichlet boundary problem.

On the other hand, if $(\lambda,\theta(\cdot,\lambda))$ is an eigenpair of Neumann boundary problem, then we have either $\theta(1/2,\lambda)=0$ or $\theta'(1/2,\lambda)=0$. This implies that $(\lambda,\theta(\cdot,\lambda))$ is an eigenpair of (3.6) or (3.5). Analogously, if $(\lambda,\varphi(\cdot,\lambda))$ is an eigenpair of Dirichlet boundary problem, then we have either $\varphi(1/2,\lambda)=0$ or $\varphi'(1/2,\lambda)=0$. This implies that $(\lambda,\varphi(\cdot,\lambda))$ is an eigenpair of (3.5) or (3.6). According to Theorem 3.3 and Theorem 4.3 in [27], we have

$$\mu_{0,V}^{NN}=\mu_0,\{\mu_{2m-1,V}^{NN},\mu_{2m-1,V}^{DD}\}\subset[\mu'_{2m-1},\mu'_{2m}],\ \{\mu_{2m,V}^{NN},\mu_{2m,V}^{DD}\}\subset[\mu_{2m-1},\mu_{2m}],$$

which leads to

$$\mu_{0,V}^{NN}=\mu_0,\{\mu_{2m-1,V}^{NN},\mu_{2m-1,V}^{DD}\}=\{\mu'_{2m-1},\mu'_{2m}\},\ \{\mu_{2m,V}^{NN},\mu_{2m,V}^{DD}\}=\{\mu_{2m-1},\mu_{2m}\}.$$

This ends the proof. □

It is now ready to formulate our main result in this paper.

Theorem 3.2. *For the characteristic Schrödinger equation* (1.1) *with symmetric 1-periodic potential* $V(x)$*, the corresponding DtN mapping can be expressed as*

$$I(z) = -\sqrt{\mu_{0,V}^{NN} - z} \prod_{m\geq 1} \frac{\sqrt{\mu_{m,V}^{NN} - z}}{\sqrt{\mu_{m,V}^{DD} - z}}, \quad \forall z \in \mathbb{C} \backslash \mathbb{R}. \tag{3.7}$$

Proof. Applying (3.4) and Theorem 3.1 we have

$$\begin{aligned}
\Delta^2(z) - 4 &= 4(\mu_0 - z) \prod_{m\geq 1} \frac{(\mu_{2m-1} - z)(\mu_{2m} - z)}{\mu_{2m,0}^{NN} \mu_{2m,0}^{DD}} \prod_{m\geq 1} \frac{(\mu'_{2m-1} - z)(\mu'_{2m} - z)}{\mu_{2m-1,0}^{NN} \mu_{2m-1,0}^{DD}} \\
&= 4(\mu_{0,V}^{NN} - z) \prod_{m\geq 1} \frac{(\mu_{2m,V}^{NN} - z)(\mu_{2m,V}^{DD} - z)}{\mu_{2m,0}^{NN} \mu_{2m,0}^{DD}} \prod_{m\geq 1} \frac{(\mu_{2m-1,V}^{NN} - z)(\mu_{2m-1,V}^{DD} - z)}{\mu_{2m-1,0}^{NN} \mu_{2m-1,0}^{DD}} \\
&= 4(\mu_{0,V}^{NN} - z) \prod_{m\geq 1} \frac{(\mu_{m,V}^{NN} - z)(\mu_{m,V}^{DD} - z)}{\mu_{m,0}^{NN} \mu_{m,0}^{DD}} = 4 t_{DD}(z) t_{NN}(z).
\end{aligned}$$

Considering $t_{ND}(z) = t_{DN}(z)$, it holds that

$$\begin{aligned}
I(z) = -\frac{t_{ND}(z) - \sigma}{t_{DD}(z)} = -\frac{\Delta(z) - 2\sigma}{2t_{DD}(z)} &= -\frac{\Delta(z)\left[1 + \sqrt{\frac{\Delta(z)-2}{\Delta(z)+2}}\right] - 2\left[1 - \sqrt{\frac{\Delta(z)-2}{\Delta(z)+2}}\right]}{2t_{DD}(z)\left[1 + \sqrt{\frac{\Delta(z)-2}{\Delta(z)+2}}\right]} \\
&= -\frac{(\Delta(z)+2)\sqrt{\frac{\Delta(z)-2}{\Delta(z)+2}}}{2t_{DD}(z)}.
\end{aligned}$$

By putting

$$\tilde{I}(z) = -\sqrt{\mu_{0,V}^{NN} - z} \prod_{m\geq 1} \frac{\sqrt{\mu_{m,V}^{NN} - z}}{\sqrt{\mu_{m,V}^{DD} - z}},$$

we derive

$$I^2(z) = \frac{\Delta^2(z) - 4}{4t_{DD}^2(z)} = \frac{t_{NN}(z)}{t_{DD}(z)} = \tilde{I}^2(z).$$

It is straightforward to verify that in the cut complex plane as the domain defined for σ, thus for I, the function $\tilde{I}$ is a holomorphic function. Since

$$\lim_{z\to-\infty} I(z) = \lim_{z\to-\infty} \tilde{I}(z) = -\infty,$$

we then derive

$$I(z) = \tilde{I}(z) = -\sqrt{\mu_{0,V}^{NN} - z} \prod_{m\geq 1} \frac{\sqrt{\mu_{m,V}^{NN} - z}}{\sqrt{\mu_{m,V}^{DD} - z}}. \tag{3.8}$$

This ends the proof. □

Remark 3.1. For Eq. (1.1) with S-periodic potential V, we can obtain the same expression (1.2) of DtN mapping I by using a simple scaling argument.

4 Second-order ODEs with periodic symmetric coefficients

Now we consider the more general second-order ODE with periodic coefficients

$$\left[-\partial_x c^{-1}(x)\partial_x + V(x)\right] y = \rho(x) z y, \tag{4.1}$$

where c and ρ are supposed to be smooth and bounded upper and below by positive numbers. If we make the variable transformation

$$x \to X = X(x) = \int_0^x \sqrt{\rho(t)c(t)}\,\mathrm{d}t,$$

and put

$$\omega = \exp\left(\frac{1}{4}\ln\frac{\rho}{c}\right) y,$$

then a direct computation yields that

$$\left[-\partial_x c^{-1}(x)\partial_x + V(x) - \rho(x)z\right] y = \rho \exp\left(-\frac{1}{4}\ln\frac{\rho}{c}\right)\left[-\partial_X^2 + \widetilde{V}(X) - z\right]\omega$$

with

$$\widetilde{V}(X) = \frac{V(x)}{\rho(x)} + \frac{1}{4}\partial_X^2 \ln\frac{\rho}{c} + \left(\frac{1}{4}\partial_X \ln\frac{\rho}{c}\right)^2.$$

Obviously, $\widetilde{V}$ is a periodic function with respect to X with the period

$$\widetilde{S} = \int_0^S \sqrt{\rho(x)c(x)}\,\mathrm{d}x.$$

If I, V and ρ are symmetric with respect to x, so is $\widetilde{V}$ with respect to X. Besides, λ is a $\widetilde{S}$-periodic or $\widetilde{S}$-antiperiodic eigenvalue of the characteristic equation

$$\left[-\partial_X^2 + \widetilde{V}(X)\right]\omega = z\omega, \tag{4.2}$$

if and only if λ is an S-periodic or S-anti-periodic eigenvalues of (4.1). Suppose $\{\mu_{m,V}^{DD}\}_{m\geq 1}$ are the Dirichlet eigenvalue of (4.1) with boundary condition $y(0)=y(S)=0$, and $\{\mu_{m,V}^{NN}\}_{m\geq 0}$ are the Neumann eigenvalues with boundary conditions $y'(0)=y'(S)=0$, then for any $z\in\mathbb{C}\backslash\mathbb{R}$, the DtN mapping of the nontrivial bounded solution of (4.2) is

$$\frac{\partial_X \omega(0)}{\omega(0)} = -\sqrt{\mu_{0,V}^{NN} - z}\prod_{m\geq 1}\frac{\sqrt{\mu_{m,V}^{NN} - z}}{\sqrt{\mu_{m,V}^{DD} - z}}.$$

The DtN mapping associated with (4.1) is then given by

$$\frac{\partial_x y(0)}{y(0)} = \sqrt{\rho(0)c(0)}\frac{\partial_X \omega(0)}{\omega(0)} = -\sqrt{\rho(0)c(0)}\sqrt{\mu_{0,V}^{NN}-z}\prod_{m\geq 1}\frac{\sqrt{\mu_{m,V}^{NN}-z}}{\sqrt{\mu_{m,V}^{DD}-z}}.$$

This is exactly the expression (1.4) which was originally formulated in [5].

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