Frequency Dependent Conductivity of the Fibonacci–Chain*

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A real–space-renormalization method for the frequency dependent conductivity of the periodic approximants of the Fibonacci chain is developed. This scheme is based on the known $2 \times 2$ transfer matrices and additional $5 \times 5$ matrices which allow an efficient numerical evaluation of the Kubo formula. Numerical results are presented.

PACS numbers: 61.44 Br, 71.23 Ft, 05.10.C

1. INTRODUCTION

Quasicrystals (QC)\(^1\) and their periodic approximants reveal unusual transport properties, e.g., extremely low conductivity for alloys of metallic constituents\(^2\), and it is generally believed that these properties are directly related to the long range but nonperiodic order. However, no coherent theoretical framework has been successfully established. For instance, previous calculations of the density of states (DOS) revealed a set of peaks and gaps of small width ($10^{-100}$meV)\(^3\) but recent studies provide convincing arguments that these structures are numerical artifacts\(^4\). Most of the previous numerical studies of the conductivity were based on the Landauer formula\(^5\) but only few studies were made in the framework of linear response theory\(^6\).

One–dimensional QCs, such as the Fibonacci chain (FC), have been studied in great detail by many researchers, because exact results and analytical treatments are possible. The most striking feature of this model is that quasiperiodicity induces long range correlations giving rise to an intermediate state of localisation. These so–called ‘critical states’ are associated to singular continuous spectra of the Hamiltonian\(^2\), while all states are

*To appear in Journal of Low Temperature Physics, March 2002
localized for randomly disordered systems in 1–D. Most progress in investigating 1–D models has been made by methods based upon the trace–map and real–space decimation techniques. To the best of our knowledge nothing comparable has been worked out for the current–current correlation function which allows for a renormalization group approach of the frequency dependent conductivity.

Our paper is organized as follows. Sec. 2 summarizes the physical model, in particular, the relation between the geometrical and the electronic structure which has been worked out in a preceding paper[7]. In Sec. 3, a suitable expression of the Kubo conductivity is derived in terms of the known $2 \times 2$ transfer matrices and additional $5 \times 5$ matrices $\Delta$, which allow to set up a real–space renormalization scheme and its numerical implementation. Sec. 4 gives some numerical results and conclusions.

2. FIBONACCI CHAIN

The FC is specified by two different types of “bonds” denoted by $L$ ("long") and $S$ ("short"), see Fig. 1. One may describe the geometric structure of such lattices by words $w(L,S)$, i.e. strings in the symbols $L,S$ representing the corresponding linear arrangement of the “letters” $L$ and $S$. These words can be generated by an (infinite) repetition of the recursion law (Nielsen transformation (NT))

$$w_n = w_{n-1} \ast w_{n-2}, \quad w_{-1} = S, \quad w_0 = L$$

where the symbol $\ast$ is defined as the concatenation of two strings and $n = 1, 2, \ldots$. The length of the FC in the $n^{th}$ generation $|w_n| = f_n$, i.e. the sum of symbols $L$ and $S$ in $w_n(L,S)$ satisfies the recursion relation for the Fibonacci numbers[8]

$$f_n = f_{n-1} + f_{n-2}, \quad f_{-1} = f_0 = 1.$$
Alternatively, the \( n \)th order approximants can be generated by substitutions (morphisms), which operate on the symbols \( L, S \) rather than on words \( w_n(L, S) \)

\[
\mathcal{L} : \begin{cases} L \mapsto LS \\ S \mapsto L \end{cases}.
\]

(3)

The mapping \( \mathcal{L} \) may be viewed as the orbit of \( L \), i.e. \( w_n = \mathcal{L}^n(L) \):

\[
L \xrightarrow{\mathcal{L}} LS \xrightarrow{\mathcal{L}} LSL \xrightarrow{\mathcal{L}} LSLLS \xrightarrow{\mathcal{L}} \ldots \xrightarrow{\mathcal{L}} LSLLSLLSL... 
\]

In our study, we employ the following tight–binding Hamiltonian

\[
\mathcal{H} = \sum_\mu |\mu > \epsilon_\mu < \mu| + \sum_{\mu, \nu} |\mu > t_{\mu, \nu} < \nu|,
\]

(4)

where \( |\mu > \) are Wannier states centered at sites \( \mu \in G = [-M, N - 1] \subseteq \mathbb{Z} \), and the real \( \epsilon_\mu, t_{\mu, \nu} \) denote the site–energies and the nearest–neighbour transfer integrals, respectively. \( (t_{\mu, \nu} > 0) \). The FC has the speciality that there is no \( S-S \) bonding, hence only three of the possible four combinations occur:

\[
\epsilon_\mu = \begin{cases} \epsilon_\alpha &: t_{\mu-1, \mu} = t_{\mu, \mu+1} = t_L, \\ \epsilon_\beta &: t_{\mu-1, \mu} = t_L, t_{\mu, \mu+1} = t_S, \\ \epsilon_\gamma &: t_{\mu-1, \mu} = t_S, t_{\mu, \mu+1} = t_L. \end{cases}
\]

(5)

To each word \( w = (y_\mu)_{\mu \in G} \equiv y_{-M} y_{-M+1} \ldots y_N \), with \( y_\mu \in \{L, S\}, M + N \geq 2 \), we uniquely assign a dual word \( \Sigma = (\sigma_\mu)_{\mu = -M}^{N-1} \equiv (\sigma_{-M}, \ldots , \sigma_{N-1}) \), where each symbol \( \sigma_\mu \in \{\alpha, \beta, \gamma\} \) will be related to the pair \( (y_\mu, y_{\mu+1}) \) by the map \( (LL, LS, SL) \leftrightarrow (\alpha, \beta, \gamma) \). For example, the dual word pertaining to \( u_5 \) is \( \Sigma^G = \gamma \beta \gamma \alpha \beta \gamma \beta \gamma \alpha \beta \gamma \alpha \), with \( G = [0, 12], \) see Fig. 1. Let be \( \Sigma_u = (\sigma_u^\mu)_{\mu = -m}^{n-1} \) and \( \Sigma_v = (\sigma_v^\mu)_{\mu = -p}^{q-1} \) the dual words of \( u \), and \( v \) respectively. We define the product of two dual words, corresponding to the product \( w = u * v \), by \( \Sigma_u \land \Sigma_v := \Sigma_w \), with \( \Sigma_w = (\sigma_w^u, \ldots, \sigma_w^{n-1}, \sigma_w, \sigma_w^v, \ldots, \sigma_w^{q-1}) \), \( \sigma_w := (y_w^u, y_w^v) \), where \( y_w^u (y_w^v) \) is the last (first) letter of \( u (v) \).

To set-up a renormalization scheme we approximate the aperiodic FC by a periodic approximant of length \( 2N (M = N) \),

\[
\Sigma^G = \underbrace{\Sigma_n \land \Sigma_n \land \ldots \land \Sigma_n}_{2N \text{times}}, \quad G = [-N, N - 1], \quad N = N' f_n,
\]

(6)

where \( f_n - 1 \) denotes the number of symbols \( \sigma_\mu \) of \( \Sigma_n \). \( c_{u} + t_{e_{u}} = e_{u}, t_{v} + t_{e_{v}} = e_{v}, \mu = \bar{\mu} + m f_n \), where \( \bar{\mu} \in [0, f_n - 1] \) labels the ‘atoms’ inside the Fibonacci supercell and \( m \in [-N', N' - 1] \) labels the vectors of the Bravais lattice.
of the periodic approximant. Obviously, there is a unique correspondence between the dual word $\Sigma$ and the FC Hamiltonian $H_{\Sigma}$.

In site representation, the eigenstates of Eq. (4) can be represented in terms of the two fundamental solutions $\{P_\mu\}$ and $\{P_{\mu-1}\}$ of the discrete Schrödinger equation

$$ (H_{\Sigma_n} \psi)_\mu := t_{\mu+1} \psi_{\mu+1}(E) + t_{\mu} \psi_{\mu-1}(E) + \epsilon_{\mu} \psi_{\mu}(E) = E \, \psi_{\mu}(E), \quad (7) $$

such that the (unnormalized) solutions are

$$ \Psi_{\mu}^\pm(E) := \mathcal{P}_\mu(E) + m_\pm(z) P_\mu(E). \quad (8) $$

$P_\mu(E), P_{\mu-1}(E)$ respectively denote polynomials of degree $\mu$ and $\mu - 1$ with initial conditions $P_{-1} = 0, P_0 = 1/t_0$ and $P_{-1} = -1/t_0, P_0 = 1$. In addition, we have to fulfill the Bloch conditions $\Psi_{\mu}^\pm f_n = \exp(\pm ika) \Psi_{\mu}$, where $a = f_n$ is the “lattice constant” and $k = k(E)$ is the wave vector. According to time–reversal symmetry a state of energy $E$ is a twofold degenerate which will be denoted by $|E, \pm\rangle$ and $\Psi_{\mu}^\pm(E) = \langle \mu | \pm \rangle$, respectively. $m_\pm(E)$ denotes the Titchmarsh–Weyl function

$$ m_{\pm}(E) = \frac{\xi_{\pm}(E) + t_0 \mathcal{P}_{f_n-1}(E)}{t_0 \mathcal{P}_{f_n-1}(E)}, \quad (9) $$

$$ \xi_{\pm}(E) := e^{\pm ik(E)f_n} = \frac{\Delta_{f_n}}{2} \pm \sqrt{\left(\frac{\Delta_{f_n}}{2}\right)^2 - 1}, \quad (10) $$

$$ \Delta_{f_n} = t_0 (P_{f_n} - \mathcal{P}_{f_n-1}); \quad (11) $$

where $f_n k(E) = (p\pi)/N' = \arccos(\Delta_{f_n}(E)/2) \in [0, \pi)$, and $0 \leq p < N'$.

For the standard one-atomic tight binding chain with equal $t'$s and $\epsilon'$s $\Delta_{f_n}(E)$ and $P_\mu(E) = \mathcal{P}_{\mu-1}$ are, apart from a scale factor, Chebyshev polynomials $T_\mu(x), U_\mu(x)$ of first and second kind, respectively. $\Psi_{\mu}^\pm(E) = e^{\pm i\mu k}, E(k) = \epsilon - 2t \cos(k)$.

### 3. CONDUCTIVITY AND REAL–SPACE RENORMALIZATION

In the linear response theory the real part of the conductivity is given by

$$ \Re \{\sigma^{(n)}(\omega)\} = \frac{\pi}{\hbar} \int_{-\infty}^{\infty} \frac{f(E) - f(E + \hbar \omega)}{\hbar \omega} \Gamma^{(n)}(E, \omega) \, dE, \quad (12) $$

$$ \Gamma^{(n)}(E, \omega) = \text{Tr} \{ \hat{J} \delta(E - \hat{H}_{\Sigma(n)}) \hat{J} \delta(E + \hbar \omega - \hat{H}_{\Sigma(n)}) \}, \quad (13) $$
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Fig. 2. Density of states (left), bandstructure (middle), and (unrestricted) solutions of Eq. (16) (right) as function of frequency. 6th order generation FC with $\epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma = 0$ and $t_L = 1.1$, $t_S = 1.0$.

where $f(E)$ is the Fermi function and $\mathbf{J}$ is the current operator

$$\mathbf{J} = \frac{ie\hbar}{m} \sum_{\mu,\nu \in G} j_{\mu\nu} |\mu\rangle \langle \nu|, \quad j_{\mu\nu} = -t_{\mu+1} \delta_{\mu\nu-1} + t_\mu \delta_{\mu\nu+1}.$$  \hfill (14)

At zero temperature and after some nontrivial algebra Eq. (12) becomes

$$\sigma^{(n)}(\omega) = -\frac{e^2}{\hbar^2 f_n} \sum_{E_\omega} \zeta \left| \frac{\text{Tr}\{\mathbf{T} \Theta \mathbf{T} \mathbf{T}^{-1} \Theta \mathbf{T}^{-1} \mathbf{T} \mathbf{T} - 2 \Theta \Theta\}}{2\omega |\Delta'_n(E) - \Delta'_n(E) - 4 + (\Delta'_n(E))^2} \right|_{E = E_\omega, \omega > 0}. \hfill (15)$$

with $\Delta' := d\Delta/dE$ and $\zeta = \text{sign}(P_{n-1}^{-1}(E)P_{n-1}(E + h\omega))$, respectively. (Note, in Eq. (13) we have omitted the dc-part $g^{(n)}(\omega)$ which vanishes in the limit $n \to \infty$). All quantities are functions of $E$ and/or $E + h\omega$ and $\mathbf{G}(E, E + h\omega) = \Theta(E + h\omega, E)$, $\mathbf{T}(E) = \mathbf{T}(E + h\omega)$, etc . . .

$E_\omega$ denotes the energy of an initial occupied (lower) band from which transitions to an empty (upper) band can take place. By conservation of energy and (crystal–) momentum $E = E_\omega$ is a solution of

$$k(E + h\omega) = k(E) \iff \Delta'_n(E + h\omega) - \Delta'_n(E) = 0.$$  \hfill (16)

Remarkably, the set of all solutions of Eq. (16), denoted by $E(\omega)$, also includes unphysical solutions which smoothly join $E_\omega$, when both $E + h\omega$ and
$E$ are in the gap regions (where $k$ is imaginary), see Fig. 2. Of course, only the subset $E_\omega$ in the spectrum of $\hat{\mathcal{H}}_{\Sigma_n}$ should be included in Eq. (13).

To evaluate Eq. (13) we introduce a matrix notation

$$T(E) \equiv T^{(n)} = t_1 \begin{pmatrix} P^{(1)}_{\tau_n} (E) & P^{(1)}_{\tau_{n-1}} (E) \\ -P^{(2)}_{\tau_n} (E) & -P^{(2)}_{\tau_{n-1}} (E) \end{pmatrix}.$$  \hspace{1cm} (17)

$P^{(\nu)}_\mu$ are the polynomials associated to $P_\mu$ which are obtained by replacing $\epsilon_\mu$, $t_\mu$ by $\epsilon_{\mu+\nu}$, $t_{\mu+\nu}$, e.g. $P_\mu = P^{(1)}_{\mu-1}$. In addition, we define $\Theta(E, E+i\omega) \equiv \Theta^{(n)}$ with

$$\Theta^{(n)} = \frac{1}{t_1} \begin{pmatrix} 2t_2 & E - \epsilon_1 \\ E - \epsilon_0 & 2t_1 \end{pmatrix} \cdot \begin{pmatrix} \Delta^{(n)}_{11} + \Delta^{(n)}_{12} & \Delta^{(n)}_{14} \\ \Delta^{(n)}_{15} & \Delta^{(n)}_{11} \end{pmatrix}.$$ \hspace{1cm} (18)

$\Delta^{(n)}_{ij}$ are components of the $5 \times 5$-matrix

$$\Delta^{(n)}(E, E+i\omega) = \Delta_{t_{n-2}} \cdot \Delta_{t_{n-3}} \cdots \Delta_1,$$ \hspace{1cm} (19)

where

$$\Delta_\mu(E, E+i\omega) = \begin{pmatrix} \bar{s}_\mu \xi_\mu + 1 & \tau_\mu \phi_\mu - \bar{s}_\mu \xi_\mu & -\tau_\mu \phi_\mu & -\tau_\mu \xi_\mu \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \bar{s}_\mu & -\bar{s}_\mu & 0 & -\tau_\mu \\ \xi_\mu & -\xi_\mu & 0 & 0 \end{pmatrix}.$$ \hspace{1cm} (20)

We have set $s_\mu = (E - \epsilon_\mu)/t_{\mu+1}$, $\bar{s}_\mu = (E + \omega - \epsilon_\mu)/t_{\mu+1}$, $\tau_\mu = t_\mu/t_{\mu+1}$, and $\zeta_\mu = s_\mu t_\mu \bar{s}_\mu + 1 t_{\mu+2} - 2t_\mu t_{\mu+1}$. Then $\xi_\mu = (\zeta_\mu s_{\mu-1} t_{\mu-1} + \zeta_{\mu-1} t_{\mu+1} + 1 t_{\mu+2})/(2\zeta_{\mu-1} t_\mu)$ and $\phi_\mu = \zeta_\mu t_{\mu-1}/\zeta_{\mu-1}$. In contrast to the matrix

$$T^{(n)} = T_{\sigma_{i_n}} \cdot T_{\sigma_{i_{n-1}}} \cdots T_{\sigma_1},$$ \hspace{1cm} (21)

which corresponds to each site $\sigma_\mu$ (i.e. to each “dual letter”, such that $T_\mu = T_{\sigma_\mu}$) uniquely, the $\Delta_\mu$ correlates three sites (i.e. a triple of three dual letters) $\sigma_{\mu-1}$, $\sigma_\mu$ and $\sigma_{\mu+1}$, respectively. Thus we may write $\Delta_\mu = \Delta_{\sigma_{\mu-1} \sigma_\mu \sigma_{\mu+1}}$, see Fig. 3.

The self similarity of FC shows up in the structure of Eqs. (13,21) which will lead to a real–space renormalization scheme of the structure of the trace–map method [13] or path renormalization used for the calculation of the local DOS [5]. To set up the renormalization scheme we consider the NT of words, cf. Eq. (13),

$$X_{1-s,s}(w_{k-1}, w_{k-2}) = (w_k, w_{k-1}), \quad w_k = (w_{k-1})^{1-s} w_{k-2} (w_{k-1})^s,$$ \hspace{1cm} (22)
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Fig. 3. Example of the RTs (24) and (28) for a 5th generation FC. Arrows indicate the dual letters $\sigma = \sigma_{\ell_n}^{(n)}$ as given by Eq. (25). $T_1 * T_2 * T_3 \equiv T_3 \cdot T_2 \cdot T_1$, etc., where the dot denotes the usual matrix–product.

with $s = 0, 1$, and the initial words $w_{-1} = S$, $w_0 = L$. Next, we write the trace–map in the form (recall, that $\Delta_{j_n} = \text{Tr}(T)$)

$$R_L(\Delta_{j_k}, \Delta_{j_{k-1}}, \Delta_{j_{k-2}}) = R_R(\Delta_{j_k}, \Delta_{j_{k-1}}, \Delta_{j_{k-2}}) = (\Delta_{j_{k+1}}, \Delta_{j_k}, \Delta_{j_{k-1}}),$$

$$\Delta_{j_{k+1}} = \Delta_{j_k} \Delta_{j_{k-1}} - \Delta_{j_{k-2}},$$  \hspace{1cm} (23)

where $L = X_{1,0}$, $R = X_{0,1}$. Note, $R_L$ is the renormalization transformation (RT) corresponding to the NT $L$ etc.. Furthermore, the quantity $\Lambda = \Delta_{j_{k-2}}^2 + \Delta_{j_{k-1}}^2 + \Delta_{j_k}^2 - \Delta_{j_{k-2}} \Delta_{j_{k-1}} \Delta_{j_k}$ is invariant under the transformation $R_L$ so that the trace–map Eq. (23) represents a dynamical system which is essentially two–dimensional. Therefore, $(\Delta_{j_{n+1}}, \Delta_{j_n}) = (R_L)^n(\Delta_{j_2}, \Delta_{j_1}).$

In addition, the NTs (22) implies

$$R_{X_{1-s_k,s_k}}(T^{(k-1)}, T^{(k-2)}) = \left((T^{(k-1)})^{s_k} T^{(k-2)} (T^{(k-1)})^{1-s_k} \right).$$ \hspace{1cm} (24)

By inspection of Eq. (21) we recognize that $T^{(n)}$ does not correspond to $\Sigma_n$ but to the cyclic permuted word $T^{(n)}(\Sigma_n) = (\sigma_1, \ldots, \sigma_{f_n})$, $\sigma_{f_n} = \sigma_0$.

The corresponding word is the word $(L, S) = \mathcal{R} \circ (\mathcal{L})^{n-1}(L)$ which implies $(T^{(n+1)}, T^{(n)}) = (R_L)^{n-1} \circ R_R (T^{(2)}, T^{(1)}).

The case of the matrices $\Delta^{(n)}$ is a little bit more involved, see Fig. 3. Let $\Delta^{(n-1)}$ and $\Delta^{(n-2)}$ correspond to the dual words $\Sigma^{(n-1)}$ and $\Sigma^{(n-2)}$, respectively. Then the NT $L$ implies $L(\Sigma_{n-1}, \Sigma_{n-2}) = (\Sigma_n, \Sigma_{n-1})$, where

$$\Sigma_n = \Sigma_{n-1} \wedge \Sigma_{n-2} \equiv (\sigma_0^{(n-1)}, \ldots, \sigma_{f_{n-1}-1}^{(n-1)}, \sigma_{f_n}^{(n-1)}, \sigma_0^{(n-2)}, \ldots, \sigma_{f_{n-2}-1}^{(n-2)}).$$ \hspace{1cm} (25)
Eq. (23) corresponds to $\Delta^{(n)} = \Delta^{(n-2)} \wedge \Delta^{(n-1)} := \Delta^{(n-2)} \cdot \delta_n \cdot \Delta^{(n-1)}$, where we have introduced a “sandwich”–matrix

$$\delta_n = \Delta_{\sigma_{f_{n-2}}^{(n-2)} \sigma_{f_{n-1}}^{(n-1)} \sigma_{f_{n-2}}^{(n-2)} \sigma_{f_{n-1}}^{(n-1)}}.$$

As a result, the NT $L$ leads to the following RT for the $\Delta^{(k)}$

$$RL\left(\Delta^{(k-1)}, \Delta^{(k-2)}\right) = \left(\Delta^{(k-2)} \cdot \delta_k \cdot \Delta^{(k-1)}\right),$$

so that $(\Delta^{(n+1)}, \Delta^{(n)}) = (RL)^n(\Delta^{(2)}, \Delta^{(1)})$ holds. Eqs. (23,24,28) provides a simple renormalization scheme to calculate the frequency dependent conductivity of the standard FC. This is our main result.

4. RESULTS AND CONCLUSIONS

Figs. 2, 4, 5 display some numerical results for the DOS, mini–bandstructure, transition energies, and the conductivity. We note, that the expression of $\sigma^{(n)}(\omega)$ in Eq. (15) is nonzero only for $\omega > 0$. For $\omega \to 0$, merely $\sigma^{(n)}(0)$ contributes because none of the lines $(E_{\omega}^{(i)}, \omega)$ cut the axis $\omega = 0$ for energies within the spectrum. Therefore, $\sigma^{(n)}(\omega)$ vanishes in the limit $\omega \to 0$. (In addition, the dc conductivity (see after Eq. (15)) vanishes in the limit of infinite aperiodic FC, $n \to \infty$.) This is characteristic for the (infinite) TB model, as $\mathcal{H}_{\Sigma n}$ is a bounded operator. Thus, there is always a gap in the neighbourhood of $\omega = 0$. If one introduces some mechanism of dissipation or disorder one may expect that the small frequency–gap revealed in Fig. 4 may be smeared out (leading to metallic–like behaviour), but will persist in the case of Fig. 5 (semiconductor–like behaviour).

The main numerical challenge turned out to be the calculation of the energies $E_{\omega}$, i.e., the zeros of Eq. (16). This task implicitly implies polynomials of very high order. Such operations are numerically unstable but could be managed with the help of Bailey’s multiprecision software packet.\(^{15}\)

Starting from the self–similarity of the FC we found a real space renormalization scheme for the Kubo–conductivity which is suitable for numerical implementation. Hereto, this scheme stands alongside with the powerful tool of the trace map for the spectrum\(^{13}\) and the path renormalisation scheme for the local DOS\(^{7}\). For details and generalizations of our approach to arbitrary morphisms (like Thue–Morse, Rudin–Shapiro, period doubling) and n-letter alphabets, we refer to Ref. 16.
Fig. 4. Density of states $N(E)$ (left) and conductivity $\sigma(\omega)$ (right) of the FC with a supercell of $f_{11} = 233$ sites. Fermi energy $\epsilon_F = 0$, $t_S = 1.0, t_L = 1.5$, and $\epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma = 0$ (arbitrary units).

Fig. 5. Density of states (left) and conductivity (right) of the same FC as in Fig. 4 but with different parameters: $\epsilon_F = -0.2, -\epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma = 1.0$.

ACKNOWLEDGMENTS

This work was supported by the Deutsche Forschungsgemeinschaft DFG through the “Schwerpunktsprogramm” Quasikristalle. D. H. Bailey and NASA Ames are kindly acknowledged for making available their Multiple Precision Floating Point Computation Package.
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14. See the Nielsen–Graph, Fig. 5, of Ref. [7]. Note, the sequence of substitutions \( L, R \) is reversed with respect to the NTs \( L, R \). Here, the path which connects \( \alpha \) and \( \sigma^{(b)} = \beta^{(b)} \) provides the sequence of NTs of the RG.

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