

## Combinatorial identities for binary necklaces from exact ray-splitting trace formulas

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Based on an exact trace formula for a one-dimensional ray-splitting system, we derive novel combinatorial identities for cyclic binary sequences (Pólya necklaces).

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### I. INTRODUCTION

Wave propagation in systems with sharp interfaces is a fundamental problem in the natural sciences and engineering. Well-known examples include light waves impinging on a water–air interface or sound waves propagating in layered media.<sup>1</sup> All these systems have one feature in common: The splitting of the incident wave into reflected and transmitted components. In the geometrical optics limit of small wave lengths, incident, reflected, and transmitted waves are described by rays. The rays are split at the interface; hence the name “ray-splitting systems”<sup>2</sup> for the whole class of wave systems with sharp interfaces. Ray-splitting systems have recently attracted attention in the context of acoustic, quantum, and electromagnetic wave chaos.<sup>2–10</sup> It was shown that the mere presence of a ray-splitting boundary can drive an otherwise regular system into chaos.<sup>2–4</sup> It was also shown that ray-splitting systems produce corrections to the Weyl formula<sup>11,12</sup> for the average density of states that can be computed analytically.<sup>5,6</sup> The most conspicuous consequence of ray splitting is the existence of non-Newtonian periodic orbits in a ray-splitting system that contribute substantially to the fluctuating part of the level density.<sup>3,4,7–9</sup> The existence of non-Newtonian orbits in a dielectric-loaded Bunimovich ray-splitting stadium was demonstrated experimentally.<sup>7–9</sup> In addition it has been shown recently that exact trace formulas exist for a class of one-dimensional ray-splitting systems.<sup>9,10</sup> These formulas were derived using results from quantum graph theory.<sup>13,14</sup> Considering the two-point correlation function of the spectra of special quantum graphs, Schanz and Smilansky were able to derive novel combinatorial identities.<sup>15</sup> This was possible by deriving the two-point correlation function in two independent ways, (i) directly using input from the quantum spectrum and (ii) using the exactness of the trace formula. Motivated by the methods of Kottos, Schanz, and Smilansky<sup>13–15</sup> we show that novel combinatorial identities for binary Pólya necklaces<sup>16,17</sup> are obtained directly by comparing the spectral density of analytically solvable quantum graphs with their exact periodic orbit expansion.

The plan of this paper is as follows: In Sec. II we present our model system, a one-dimensional ray-splitting system, whose spectrum can be obtained analytically. We present an exact periodic-orbit expansion of its level density expressed as a generalized Fourier sum over binary Pólya necklaces. In Sec. III we outline our method for obtaining exact combinatorial identities for binary necklaces derived from analytically solvable cases of the one-dimensional ray-splitting system. In Sec. IV we present two worked examples that yield two infinite sets of combinatorial identities. In Sec. V we discuss our results and conclude the paper.

### II. SPECTRUM

Denote by  $E_n$  the spectrum of the one-dimensional scaled Schrödinger equation

$$-\psi''(x) + V_\lambda(E, x)\psi(x) = E\psi(x), \quad (1)$$

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where

$$V_\lambda(E,x) = \begin{cases} 0, & \text{for } 0 < x \leq a \\ \lambda E, & \text{for } a < x < 1, \\ \infty, & \text{for } x \notin (0,1) \end{cases} \tag{2}$$

and  $\psi(x) \equiv 0$  for  $x \notin (0,1)$ . Scaling potentials of the form (2) arise naturally in many ray-splitting systems, for instance in dielectric-loaded cavities.<sup>5,7-9</sup> In this paper we concentrate on the case  $E > V_\lambda(E,x)$  for all  $x$ . Then, without restriction of generality, the scaling constant  $\lambda$  can be assumed to satisfy  $0 \leq \lambda < 1$ . Define  $E = k^2$ , then the spectrum of (1) is determined by

$$\sin[k(\sigma_L + \sigma_R)] - r \sin[k(\sigma_L - \sigma_R)] = 0, \tag{3}$$

where  $\sigma_L = a$ ,  $\sigma_R = \eta(1 - a)$ ,  $\eta = \sqrt{1 - \lambda}$ , and  $r = (1 - \eta)/(1 + \eta)$  is the reflection coefficient. For the derivations below it is useful to define the transmission coefficient  $t = \sqrt{1 - r^2}$ . Therefore, the reflection and transmission coefficients satisfy the relation

$$r^2 + t^2 = 1. \tag{4}$$

Since in this paper we focus on the case  $0 \leq \lambda < 1$ , both  $r$  and  $t$  are real and positive and range between 0 and 1. Possible quantum phases incurred at reflection or transmission events are treated explicitly and separately [see, e.g., (6) below]. They are not included in  $r$  or  $t$ .

We now discuss an alternative method of solving the quantum dynamics in the potential (2). This method is based on coding the periodic orbits with the help of symbol strings. We denote a bounce off  $x = 0$  by the letter  $\mathcal{L}$  and a bounce off  $x = 1$  by the letter  $\mathcal{R}$ . Words formed with these two letters code for periodic orbits in (2). The word  $\mathcal{L}$ , for instance, codes for the non-Newtonian orbit that bounces between  $x = 0$  and  $x = a$  (above-barrier reflection orbit). The word  $\mathcal{LR}$  codes for the (Newtonian) orbit that bounces between  $x = 0$  and  $x = 1$ . Since a periodic orbit represented by the word  $w$  cycles through the letters of  $w$  without a well-defined beginning or end, two words  $w$  and  $w'$  are equivalent in our context, and code for the same periodic orbit, if they are of the same length (i.e., they consist of the same number of symbols) and their respective symbol sequences are identical up to cyclic permutations. Sequences of objects that are identical up to cyclic permutations are called (Pólya) necklaces.<sup>16,17</sup> If the number of objects they consist of is two, they are called binary necklaces. Apparently, therefore, the periodic orbits of (2) can be coded with the help of binary necklaces over the symbols  $\mathcal{L}$  and  $\mathcal{R}$ . It is remarkable that for (2) every Newtonian or non-Newtonian periodic orbit can be mapped one-to-one onto a binary necklace. In other words, “pruning” is not necessary for the binary necklaces relevant for (2). Every binary necklace defines a possible periodic orbit of (2) and vice versa.

Given two letters, for instance  $\mathcal{L}$  and  $\mathcal{R}$ , we can form  $2^\ell$  words of length  $\ell$ . But, in general, many of these words will be cyclically equivalent, and correspond to the same necklace. So, how many necklaces of length  $\ell$  are there? This question is answered by the following formula. There are exactly<sup>17</sup>

$$N(\ell) = \frac{1}{\ell} \sum_{n|\ell} \phi(n) 2^{\ell/n}, \tag{5}$$

binary necklaces of length  $\ell$ , where the symbol “ $n|\ell$ ” denotes “ $n$  is a divisor of  $\ell$ ,” and  $\phi(n)$  is Euler’s totient function defined as the number of positive integers smaller than  $n$  and relatively prime to  $n$  with  $\phi(1) = 1$  as a useful convention. Thus the first four totients are given by  $\phi(1) = 1$ ,  $\phi(2) = 1$ ,  $\phi(3) = 2$ , and  $\phi(4) = 2$ . We illustrate (5) with two examples for  $\ell = 1$  and  $\ell = 2$ . There are two necklaces for  $\ell = 1$ ,  $\mathcal{L}$  and  $\mathcal{R}$ . Applying (5) to this problem, we verify  $N(1) = \phi(1) \times 2 = 2$ . There are three necklaces of length 2,  $\mathcal{LL}$ ,  $\mathcal{LR}$ , and  $\mathcal{RR}$ ; again verified by (5),  $N(2) = [\phi(1) \times 4 + \phi(2) \times 2] / 2 = 3$ .

Given a binary necklace  $w$ , we define the following integer-valued functions on  $w$ :  $n_{\mathcal{R}}(w)$  counts the number of  $\mathcal{R}$ s in  $w$ ,  $n_{\mathcal{L}}(w)$  counts the number of  $\mathcal{L}$ s,  $n(w) = n_{\mathcal{L}}(w) + n_{\mathcal{R}}(w)$ ,  $\chi(w)$  is the sum of  $n(w)$  and the number of  $\mathcal{R}$ -pairs in  $w$ ,  $\alpha(w)$  counts all occurrences of  $\mathcal{R}$ -pairs or  $\mathcal{L}$ -pairs,  $\beta(w)$  counts all occurrences of  $\mathcal{RL}$  or  $\mathcal{LR}$  and  $\gamma(w)$  is defined as  $\gamma(w) = 2n_{\mathcal{L}}(w) + n_{\mathcal{R}}(w)$ . Note that the counting of  $\mathcal{R}$ -pairs,  $\mathcal{L}$ -pairs,  $\mathcal{LR}$ - or  $\mathcal{RL}$ -combinations is to be understood cyclically, i.e., for example,  $\alpha(\mathcal{R}) = 1$  and  $\beta(\mathcal{LR}) = 2$ . Next we define the set  $W_p$  of prime necklaces as the ones that cannot be written as a periodic concatenation of substrings. As shown recently,<sup>10</sup> there exists an exact periodic orbit expansion for the spectral density of (1) in terms of prime binary necklaces

$$\rho(k) = \bar{\rho} + \frac{1}{2\pi} \sum_{w \in W_p} S_w \sum_{\substack{\nu=-\infty \\ \nu \neq 0}}^{\infty} [(-1)^{\chi(w)} r^{\alpha(w)} t^{\beta(w)}]^{|\nu|} e^{i\nu S_w k}, \quad k > 0, \tag{6}$$

where

$$S_w = 2[n_{\mathcal{R}}(w)\sigma_R + n_{\mathcal{L}}(w)\sigma_L], \tag{7}$$

is the action of the primitive periodic orbit coded by the prime binary necklace  $w$  and  $\bar{\rho} = (\sigma_L + \sigma_R)/\pi$  is the average level density.

### III. METHOD

For special values of the parameters of the potential well (2) it is possible to solve (3) analytically, thus obtaining directly the density of states  $\rho(k)$ . Equating the explicit expression for  $\rho(k)$  with the necklace expansion (6), one obtains combinatorial identities for binary necklaces. An illustrative example is the case  $a = 1$ , for which the spectral density of (1) is given by

$$\rho(k) = \sum_{m=-\infty}^{\infty} \delta(k - \pi m). \tag{8}$$

In this case there exists only one primitive necklace,  $\mathcal{LR}$ , and the necklace expansion of (6) yields

$$\rho(k) = \frac{1}{\pi} \sum_{\nu=-\infty}^{\infty} e^{2i\nu k}. \tag{9}$$

Equating (8) and (9) yields the well-known Poisson formula.

A comment is in order here. For every finite  $a$  the necklace expansion (6) involves an infinite sum over prime periodic necklaces. At  $a = 1$  this sum collapses to a single term. One may ask the question how this singular limit arises. The answer is the following. For every finite  $a$  the actions of the right-hand lobes of the periodic orbits of (6) is finite. At  $a = 1$ , these actions are zero. Consequently, all necklaces that represent *different* prime periodic orbits for  $a \neq 1$  become *repetitions* of the Newtonian periodic orbit  $\mathcal{LR}$  at  $a = 1$ . This is the reason for the existence of only a single prime periodic orbit ( $\mathcal{LR}$ ) at  $a = 1$ .

Apart from trivial and well-known identities such as (8) and (9) above, (6) is a rich source of new and nontrivial combinatorial identities for binary necklaces. Specific examples are discussed in Sec. III. Here we outline the general method.

Equation (3) can be written as

$$\sin(\omega_1 k) - r \sin(\omega_2 k) = 0, \tag{10}$$

where  $\omega_1 = \sigma_L + \sigma_R$  and  $\omega_2 = \sigma_L - \sigma_R$ . A negative  $\omega_2$  corresponds to a mirror reflection of  $V_{\lambda}(E, x)$  with respect to  $x = 1/2$ . Thus, because of  $\sigma_L, \sigma_R \geq 0$ , and without loss of generality, we may assume  $\omega_1 \geq \omega_2 \geq 0$ .

In case  $\omega_1$  and  $\omega_2$  are rationally related, i.e.,  $\omega_1/\omega_2 = p/q$ ,  $p \geq q \in \mathbb{N}$  and  $p, q$  relatively prime, (10) is reduced to the algebraic equation

$$\sin(p\omega k) - r \sin(q\omega k) = 0, \tag{11}$$

where  $\omega_1 = p\omega$  and  $\omega_2 = q\omega$ . Using the formula

$$\sin(nx) = \sin(x)U_{n-1}(\cos(x)), \tag{12}$$

where  $U_{n-1}(x)$  is the Chebyshev polynomial of the second kind, one obtains

$$\sin(\omega k)[U_{p-1}(\cos \omega k) - rU_{q-1}(\cos \omega k)] = 0. \tag{13}$$

It follows immediately from (13) that in the case of rationally related  $\omega_1$  and  $\omega_2$  there always exists a sequence of roots  $k_n^{(0)} = \pi n/\omega$ . The remaining roots are determined by

$$U_{p-1}(x) - rU_{q-1}(x) = 0, \tag{14}$$

where  $x = \cos(\omega k)$ . Since every root  $x_j$  of (14) gives rise to a periodic sequence of eigenvalues,  $\cos(\omega k_n^{(j)}) = x_j$ ,  $j = 1, 2, \dots, p-1$ , together with the sequence  $k_n^{(0)}$  the spectrum of (10) consists of  $p$  (possibly degenerate) periodic sequences of roots. Whenever (14) can be solved analytically, the density of states

$$\rho(k) = \sum_{j=0}^{p-1} \sum_{n=-\infty}^{\infty} \delta(k - k_n^{(j)}), \tag{15}$$

is known explicitly and together with (6) leads to a host of combinatorial identities for binary necklaces. Two examples are presented in the following section.

#### IV. COMBINATORIAL IDENTITIES

*Example 1:* For  $\sigma_L = \sigma_R$  equation (3) becomes

$$\sin(2ka) = 0, \tag{16}$$

with the solutions  $k_n = \pi n/(2a)$ . Note that there is no  $r$ -dependence in (16). The density of states is given by

$$\rho(k) = \sum_{n=-\infty}^{\infty} \delta\left(k - \frac{\pi n}{2a}\right) = \frac{2a}{\pi} \sum_{m=-\infty}^{\infty} e^{4imka}. \tag{17}$$

According to (7) and due to  $\sigma_L = \sigma_R$ ,  $S_w$  depends only on the binary length of  $w$  and is given by  $S_w = 2an(w)$ . Thus the sum (6) can be written as

$$\rho(k) = \frac{2a}{\pi} + \frac{a}{\pi} \sum_{\substack{m=-\infty \\ m \neq 0}}^{\infty} \sum_{w \cdot \nu \in W_{|m|}} n(w)[(-1)^{\chi(w)} r^{\alpha(w)} t^{\beta(w)}]^{\nu} e^{2imka}, \tag{18}$$

where  $W_n$  denotes the set of all length- $n$  binary necklaces  $w$ ,  $w$  is the shortest primitive code-piece in  $w$  and  $\nu$  is the number of its repetitions in  $w$ . Comparing the series (17) and (18), we see that odd-length and even-length binary necklaces satisfy the sum rules

$$\sum_{w \cdot \nu \in W_{2m-1}} n(w)[(-1)^{\chi(w)} r^{\alpha(w)} t^{\beta(w)}]^{\nu} = 0, \quad m = 1, 2, \dots \tag{19}$$

and

TABLE I. List of the three cyclically nonequivalent binary necklaces of length 2 together with their primitives ( $w$ ) and repetition indices ( $\nu$ ). Some properties of the primitives, such as their lengths ( $n$ ), number of  $\mathcal{R}$  or  $\mathcal{L}$  pairs ( $\alpha$ ), number of transmissions ( $\beta$ ), their weighted lengths ( $\gamma$ ) and their phases ( $\chi$ ) are also listed.

$j$	$w_j$	$w_j$	$\nu_j$	$n(w_j)$	$\alpha(w_j)$	$\beta(w_j)$	$\gamma(w_j)$	$\chi(w_j)$
1	$\mathcal{L}\mathcal{L}$	$\mathcal{L}$	2	1	1	0	2	1
2	$\mathcal{L}\mathcal{R}$	$\mathcal{L}\mathcal{R}$	1	2	0	2	3	2
3	$\mathcal{R}\mathcal{R}$	$\mathcal{R}$	2	1	1	0	1	2

$$\frac{1}{2} \sum_{w \cdot \nu \in W_{2m}} n(w) [(-1)^{\chi(w)} r^{\alpha(w)} t^{\beta(w)}]^\nu = 1, \quad m = 1, 2, \dots \tag{20}$$

At first glance it may seem surprising that (20) is a constant for all  $r$ . The solution lies in the relation (4). When properly ordered according to powers of  $r$  and  $t$ , it turns out that (i) individual terms in (20) are of the form  $r^{2p}t^{2q}$ , where  $p + q = m$  and (ii) the coefficients in front of the term  $r^{2p}t^{2q}$  in (20) turn out to be binomial coefficients. Thus, for given  $m$ , the left-hand side of (20) reduces to  $(r^2 + t^2)^m$ , which, according to (4) is equal to 1 for any choice of  $r$ . This explains why the seemingly variable left-hand side of (20) is nevertheless a constant. Thus we obtain from (20) the following infinite set of combinatorial identities for even-length binary necklaces:

$$\frac{1}{2} \sum_{w \cdot \nu \in W_{2m}} n(w) (-1)^{\nu \cdot \chi(w)} \delta_{\nu \cdot \alpha(w)/2, s} = \binom{m}{s}, \quad s = 0, \dots, m, \quad m = 1, 2, \dots, \tag{21}$$

where  $\delta_{i,j}$  is the Kronecker symbol.

In order to illustrate (21) let us first focus on the case  $m = 1$ . According to (5) there are exactly three cyclically nonequivalent necklaces of binary length 2 given by  $w_1 = \mathcal{L}\mathcal{L}$ ,  $w_2 = \mathcal{L}\mathcal{R}$ ,  $w_3 = \mathcal{R}\mathcal{R}$ . The necklaces  $w_1$  and  $w_3$  are not primitive. The necklace  $w_1$  is a twofold repetition of the primitive necklace  $w_1 = \mathcal{L}$ . Thus  $\nu_1 = 2$ . An analogous consideration for  $w_3$  yields  $w_3 = \mathcal{R}$  and  $\nu_3 = 2$ . The necklace  $w_2$  is primitive. Therefore,  $w_2 = w_2 = \mathcal{L}\mathcal{R}$  and  $\nu_2 = 1$ . The three necklaces  $w_j$ ,  $j = 1, 2, 3$ , are listed in Table I. Also listed are their primitives  $w_j$ , the repetition indices  $\nu_j$ , and the values of the functions  $n(w_j)$ ,  $\alpha(w_j)$ ,  $\beta(w_j)$ ,  $\gamma(w_j)$ , and  $\chi(w_j)$ .

We are now ready to check (21). For  $m = 1$  we have two choices for  $s$ :  $s = 0$  and  $s = 1$ . For  $s = 0$  we have to scan the three words  $w_j$ ,  $j = 1, 2, 3$ , for  $\nu_j \alpha(w_j)/2 = s = 0$ . According to the entries in Table I, only  $w_2$  qualifies and the sum on the left-hand side of (21) reduces to the single term

$$\frac{1}{2} n(w_2) (-1)^{\nu_2 \chi(w_2)} = 1 = \binom{1}{0}. \tag{22}$$

This shows that (21) is indeed true for the simplest case  $m = 1$ ,  $s = 0$ . For the case  $m = 1$ ,  $s = 1$  we have to check Table I for occurrences with  $\nu_j \alpha(w_j)/2 = 1$ . This is fulfilled for the necklaces  $w_1$  and  $w_3$ . We obtain

$$\frac{1}{2} [n(w_1) (-1)^{\nu_1 \chi(w_1)} + n(w_3) (-1)^{\nu_3 \chi(w_3)}] = 1 = \binom{1}{1}. \tag{23}$$

This shows that (21) also works for  $m = 1$ ,  $s = 1$ .

Testing (21) for  $m = 2$  involves finding all nonequivalent necklaces of binary length 4. According to (5) there are exactly six. All six necklaces are listed in Table II together with their properties. For  $m = 2$  we have three possibilities for  $s$ :  $s = 0, 1, 2$ . For  $s = 0$  we have to check Table II for necklaces that fulfill  $\nu_j \alpha(w_j)/2 = 0$ . Only  $w_4$  qualifies. We obtain  $n(w_4)/2 = 1$ , which equals  $\binom{2}{0}$ , the binomial coefficient on the right-hand side of (21). For  $s = 1$  we have to check for  $\nu_j \alpha(w_j)/2 = 1$ . We find three candidates:  $w_2$ ,  $w_3$ , and  $w_5$ . This time we have to be careful when summing the three terms on the left-hand side of (21), since  $\nu_3 \chi(w_3) = 5$ . Therefore, the second

TABLE II. List of the six cyclically nonequivalent binary necklaces of length 4. The meaning of the columns is the same as in Table I.

$j$	$w_j$	$w_j$	$v_j$	$n(w_j)$	$\alpha(w_j)$	$\beta(w_j)$	$\gamma(w_j)$	$\chi(w_j)$
1	$\mathcal{L}\mathcal{L}\mathcal{L}\mathcal{L}$	$\mathcal{L}$	4	1	1	0	2	1
2	$\mathcal{L}\mathcal{L}\mathcal{L}\mathcal{R}$	$\mathcal{L}\mathcal{L}\mathcal{L}\mathcal{R}$	1	4	2	2	7	4
3	$\mathcal{L}\mathcal{L}\mathcal{R}\mathcal{R}$	$\mathcal{L}\mathcal{L}\mathcal{R}\mathcal{R}$	1	4	2	2	6	5
4	$\mathcal{L}\mathcal{R}\mathcal{L}\mathcal{R}$	$\mathcal{L}\mathcal{R}$	2	2	0	2	3	2
5	$\mathcal{L}\mathcal{R}\mathcal{R}\mathcal{R}$	$\mathcal{L}\mathcal{R}\mathcal{R}\mathcal{R}$	1	4	2	2	5	6
6	$\mathcal{R}\mathcal{R}\mathcal{R}\mathcal{R}$	$\mathcal{R}$	4	1	1	0	1	2

term in (21) contributes with a minus sign. We obtain  $[n(w_2) - n(w_3) + n(w_5)]/2 = 2$ , which equals  $\binom{2}{1}$ , the corresponding binomial coefficient on the right-hand side of (21). Two necklaces,  $w_1$  and  $w_6$ , contribute in the case  $s = 2$  and again satisfy (21).

*Example 2:* Suppose now that  $\sigma_L = 2\sigma_R$ . In this case (3) becomes

$$\sin(ka/2)[4 \cos^2(ka/2) - r - 1] = 0. \tag{24}$$

This equation has three sets of solutions

$$k_n^{(j)} = \frac{2j}{a} \arccos(\varphi) + \frac{2\pi n}{a}, \quad j = -1, 0, 1, \tag{25}$$

where  $\varphi = \sqrt{1 + r/2}$ . The density of states is

$$\begin{aligned} \rho(k) &= \sum_{j=-1}^1 \sum_{m=-\infty}^{\infty} \delta\left(k + \frac{2j}{a} \arccos(\varphi) - \frac{2\pi m}{a}\right) \\ &= \frac{a}{2\pi} \sum_{j=-1}^1 \sum_{n=-\infty}^{\infty} e^{in[ak + 2j \arccos(\varphi)]} \\ &= \frac{a}{2\pi} \sum_{n=-\infty}^{\infty} e^{inak} [2T_{2n}(\varphi) + 1], \end{aligned} \tag{26}$$

where  $T_n(x) \equiv \cos(n \arccos x)$  are the Chebyshev polynomials of the first kind.<sup>18</sup> Equating (26) order-by-order with the necklace expansion (6) we obtain the sum rules

$$\begin{aligned} &\sum_{w \in W_p} \sum_{\nu=1}^{\infty} \gamma(w) [(-1)^{\chi(w)} r^{\alpha(w)} (1 - r^2)^{\beta(w)/2}]^{\nu} \delta_{\nu \gamma(w), m} \\ &= 1 + \sum_{j=0}^m \frac{2m(-1)^j}{2m-j} \binom{2m-j}{j} (1+r)^{m-j}, \quad m = 1, 2, \dots \end{aligned} \tag{27}$$

We used formula 22:6:1 of Ref. 18 for the Chebyshev polynomials in (26).

Ordering (27) according to powers of  $r$ , (27) can be reformulated as a combinatorial theorem on the set of binary necklaces, in which  $\mathcal{L}$  beads weigh twice as much as  $\mathcal{R}$  beads:

$$\begin{aligned} &\sum_{w \in W_p, C} \gamma(w) (-1)^{[2m\chi(w) + s\gamma(w) - m\alpha(w)]/[2\gamma(w)]} \left( \frac{\frac{m\beta(w)}{2\gamma(w)}}{\frac{s\gamma(w) - m\alpha(w)}{2\gamma(w)}} \right) \\ &= \delta_{s,0} + \sum_{j=0}^{m-s} \frac{2m(-1)^j}{2m-j} \binom{2m-j}{j} \binom{m-j}{s}, \quad s = 0, 1, \dots, m, \quad m = 1, 2, \dots \end{aligned} \tag{28}$$

The condition  $C$  in the sum (28) is  $C = \gamma(w) |m \wedge s - m\alpha(w)| / \gamma(w)$  even. The sum on the left-hand side of (28) may be empty. In this case the sum is defined to be zero.

Let us check (28) with the help of a few examples. First we focus on the case  $m=1, s=0$ . In order to fulfill the first part of the condition  $C$  in (28) we need  $\gamma=1$ . This, in turn, requires to find a necklace with  $n_{\mathcal{L}}=0$  and  $n_{\mathcal{R}}=1$ . There is just one such necklace, namely  $\mathcal{R}$ . But it does not fulfill the second part of  $C$ . Therefore, the sum on the left-hand side of (28) is empty, and the left-hand side is zero. The right-hand side adds up to  $1+1-2=0$  and confirms (28) for this special case. For  $s=1$  we find again that  $\mathcal{R}$  is the only choice for  $w$ . But this time the second part of  $C$  is fulfilled and the left-hand side of (28) is

$$\gamma(\mathcal{R})(-1)^{[2\chi(\mathcal{R})+\gamma(\mathcal{R})-\alpha(\mathcal{R})]/[2\gamma(\mathcal{R})]} \left( \frac{\beta(\mathcal{R})/[2\gamma(\mathcal{R})]}{[\gamma(\mathcal{R})-\alpha(\mathcal{R})]/[2\gamma(\mathcal{R})]} \right) = 1. \quad (29)$$

We used  $\alpha(\mathcal{R})=1, \beta(\mathcal{R})=0, \gamma(\mathcal{R})=1$ , and  $\chi(\mathcal{R})=2$ . For  $m=1, s=1$  the right-hand side of (28) consists of just one term, which turns out to be 1 as well. Thus we checked that (28) works for  $m=1$ . With the help of Tables I and II, other special cases may be checked as well.

## V. DISCUSSION AND CONCLUSIONS

The work presented here is closely related to the theory of quantum graphs.<sup>13–15</sup> While the quantum graphs considered by Kottos, Schanz, and Smilansky<sup>13–15</sup> correspond to the case of zero potential on the bonds and delta potentials on the vertices, the step potentials considered in this paper correspond to constant potentials on the bonds and potential steps at the vertices. Thus, although the methods employed in this paper are essentially those used previously by Kottos, Schanz, and Smilansky, we obtain a different class of combinatorial identities that apply to cyclic binary codes (Pólya necklaces). Another difference concerns the derivation of identities. While Kottos, Schanz, and Smilansky use a route that involves two-point correlation functions, we show that novel combinatorial identities can be obtained directly from the periodic orbit expansions of explicitly solvable cases. These minor differences notwithstanding the central idea for generating entirely new classes of combinatorial identities is the same: Combinatorial identities can be obtained whenever a quantum system admits of (i) an explicit analytical solution and (ii) an exact periodic orbit expansion.

In addition to the two examples presented above, there exist many other cases in which (14) can be reduced to a low-order polynomial that can be solved by elementary means. Examples are the cases  $p=3, q=2$  or  $p=5, q=3$ . Both cases can be treated in complete analogy to Example 2 above, and result in novel sum rules and combinatorial identities.

Recently we proved<sup>10</sup> that exact trace formulas exist for one-dimensional square wells with an arbitrary number of potential steps inside. Following the methods outlined above, our results can be generalized immediately to obtain novel combinatorial identities for necklaces with more than two types of beads.

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