

## REAL ZEROS OF DEDEKIND ZETA FUNCTIONS OF REAL QUADRATIC FIELDS

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ABSTRACT. Let  $\chi$  be a primitive, real and even Dirichlet character with conductor  $q$ , and let  $s$  be a positive real number. An old result of H. Davenport is that the cycle sums  $S_\nu(s, \chi) = \sum_{n=\nu q+1}^{(\nu+1)q-1} \frac{\chi(n)}{n^s}$ ,  $\nu = 0, 1, 2, \dots$ , are all positive at  $s = 1$ , and this has the immediate important consequence of the positivity of  $L(1, \chi)$ . We extend Davenport's idea to show that in fact for  $\nu \geq 1$ ,  $S_\nu(s, \chi) > 0$  for all  $s$  with  $1/2 \leq s \leq 1$  so that one can deduce the positivity of  $L(s, \chi)$  by the nonnegativity of a finite sum  $\sum_{\nu=0}^t S_\nu(s, \chi)$  for any  $t \geq 0$ . A simple algorithm then allows us to prove numerically that  $L(s, \chi)$  has no positive real zero for a conductor  $q$  up to 200,000, extending the previous record of 986 due to Rosser more than 50 years ago. We also derive various estimates explicit in  $q$  of the  $S_\nu(s, \chi)$  as well as the shifted cycle sums  $T_\nu(s, \chi) := \sum_{n=\nu q + \lfloor q/2 \rfloor + 1}^{(\nu+1)q + \lfloor q/2 \rfloor} \frac{\chi(n)}{n^s}$  considered previously by Leu and Li for  $s = 1$ . These explicit estimates are all rather tight and may have independent interests.

### 1. INTRODUCTION

Let  $\chi$  be a primitive real Dirichlet character. It is a fundamentally difficult and profound problem to show that the Dirichlet  $L$ -function  $L(s, \chi) := \sum_{n=1}^{\infty} \frac{\chi(n)}{n^s}$  is nonvanishing for real  $s > 0$ . In the case of odd character  $\chi(-1) = -1$ , which corresponds to the imaginary quadratic field, the  $L$  series can be related to Epstein zeta functions of positive definite binary quadratic forms which have rapidly converging expansions (see [1] and [10]) and in 1968 M. Low [6] devised a method which allowed him to show that  $L(s, \chi) > 0$  for  $s > 0$  for a negative conductor up to -593,000. Recently this has been corrected and extended by M. Watkins [13] to -300,000,000. Apparently, only recently in [2] has the positivity of  $L(s, \chi)$  throughout  $s \in [1/2, 1]$  been proven for an infinite number of primitive Dirichlet  $L$  functions by Conrey and Soundararajan. They proved that this holds for at least 20% of the primitive odd characters of conductor  $-8d$  for positive odd square-free  $d$ .

On the other hand, little seems to have been done in the case of even character  $\chi(-1) = 1$ . Apparently the best published method is that of Rosser, who showed, more than 50 years ago in [7] and in an unpublished work that  $L(s, \chi)$  has no real positive zero for a positive conductor up to 986.

In this note we extend an old idea of H. Davenport [3] and give a simple computational method for showing the nonvanishing of  $L(s, \chi)$  for real positive  $s$  for even real primitive characters. Our key observation is that the partial cycle sums

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$S_\nu(s, \chi) = \sum_{n=\nu q+1}^{(\nu+1)q-1} \frac{\chi(n)}{n^s}$  are positive for  $1/2 \leq s \leq 1$  and  $\nu = 1, 2, 3, \dots$ . This extends Davenport's observation from  $s = 1$ . It implies that if we can show that an exact finite sum  $\sum_{\nu=0}^t S_\nu(s, \chi)$  is nonnegative for some  $t \geq 0$ , then we can deduce  $L(s, \chi) > 0$  for the fixed  $s$ . A simple idea using the mean value theorem allows us to extend this to an algorithm for verifying the nonvanishing of  $L(s, \chi)$  for  $1/2 \leq s \leq 1$  (see ALGO 1 in subsection 2.2). By the functional equation [4] and the easy fact that  $L(s, \chi) \neq 0$  for  $\operatorname{Re}(s) > 1$ , we are able to verify numerically the following result:

**Theorem 1.1.** *Let  $\chi$  be a real and even primitive Dirichlet character with conductor  $q$ . Then  $L(s, \chi)$  has no real positive zero for  $q \leq 200,000$ .*

Since  $\zeta_{\mathbf{Q}(\sqrt{q})}(s) = \zeta(s)L(s, \chi)$ , this implies that the corresponding Dedekind zeta functions have no positive real zero. The reader with more computing power should be able to extend the range of  $q$  in Theorem 1.1 using our method. In subsection 2.1, we give the key result: Theorem 2.1, which is the extension of Davenport's result but we also give estimates for the partial cycle sum explicit in  $q$ . The algorithm used for verifying positivity and a discussion of some possible extensions is given in subsection 2.2. Proofs of our results and the estimates are given in Section 3 while Section 4 contains further estimates extending results of Leu and Li [5] who generalized Davenport's idea to shifted cycle sums. Theorem 4.1 is an analogue of Theorem 2.1. Finally in Section 5 we give the results of our numerical computations.

## 2. MAIN IDEAS AND RESULTS

**2.1. An extension of a result of Davenport.** Let  $\chi$  be a primitive Dirichlet character mod  $q$ . We define for any real  $s > 0$ ,

$$(2.1) \quad S_\nu(s, \chi) := \sum_{n=\nu q+1}^{(\nu+1)q} \frac{\chi(n)}{n^s}, \quad \nu = 0, 1, 2, \dots$$

In 1949, in response to a question of Erdős, H. Davenport proved, "with little difficulty" [3] that if  $\chi$  is real and even,  $S_\nu(1, \chi) > 0$  for all  $\nu \geq 0$ . By continuity, one expects that this should extend to a small neighborhood (depending on  $q$ ) to the left of  $s = 1$  but one does not expect to be able to prove this easily because of obvious implications to the question of Siegel's zero [9], [11]. However one can easily extend Davenport's arguments to prove the following.

**Theorem 2.1.** *If  $\chi$  is real, primitive and even, and  $1/2 \leq s \leq 1$ , then we have*

$$(2.2) \quad S_\nu(s, \chi) > 0, \quad \text{for } \nu = 1, 2, 3, \dots$$

*More precisely, we have the following explicit lower bounds for  $1/2 \leq s \leq 1$ :*

$$(2.3) \quad S_1(s, \chi) > \frac{s}{40q^{s-1/2}} \left( 1 - \frac{5}{2^{s+3}} \right),$$

$$(2.4) \quad S_\nu(s, \chi) > \frac{s}{40q^{s-1/2}} \left( \frac{1}{\nu^{1+s}} - \frac{1}{(\nu+1)^{1+s}} \right), \quad \text{for } \nu = 2, 3, \dots$$

In view of (2.2), we define for  $t = 0, 1, 2, 3, \dots$ ,

$$(2.5) \quad L_t(s, \chi) := \sum_{\nu=0}^t S_\nu(s, \chi),$$

which increases monotonically and converges to  $L(s, \chi)$ . By (2.2) it suffices for us to show that  $L_t(s, \chi) \geq 0$  for any  $t \geq 0$  to conclude that  $L(s, \chi) > 0$ . By the Extended Riemann Hypothesis, such a finite  $t$  must exist. Indeed in most cases, it suffices to choose  $t = 0$ . In fact  $L_t(s, \chi)$  converges rapidly to  $L(s, \chi)$  for any primitive characters (not necessarily real or even). Let us set

$$L(s, \chi) = L_t(s, \chi) + E_{t+1}(s, \chi).$$

Then we have the following explicit bound for the error:

**Theorem 2.2.** *Let  $\chi$  be any primitive character mod  $q$  and  $s > 0$ . Then we have*

$$(2.6) \quad |E_{t+1}(s, \chi)| \leq \frac{1}{q^{s-1/2}} \left( \frac{s}{12(t+1)^{s+1}} + \frac{s(s+1)(s+2)}{720(t+1)^{s+3}} \right) \quad \text{if } \chi \text{ is even,}$$

$$(2.7) \quad |E_{t+1}(s, \chi)| \leq \frac{1}{q^{s-1/2}} \left( \frac{|L(1, \chi)|}{\pi(t+1)^s} + \frac{s(s+1)\zeta(3)}{4\pi^3(t+1)^{s+2}} \right), \quad \text{if } \chi \text{ is odd.}$$

Let us say that a primitive modulus  $q$  for a real even character is exceptional for  $s, s \in [0, 1]$  if  $S_0(s, \chi) < 0$ . Davenport’s result is that there is no exceptional  $q$  for  $s = 1$  and we expect this to remain true for  $s$  near 1. Numerically, we have found that up to 1,000,000, there is no exceptional  $q$  for  $s = 0.555$  or  $0.56$  and there are only two at 14,693 and 788,933 at  $s = 0.55$ . Indeed it may be the case that exceptional  $q$  does not exist for  $s > 0.555$ . Indeed for all the  $q$  values up to 200,000 that we consider which are exceptional for  $s = 1/2$ , we have verified numerically that  $S_0(s, \chi)$  is increasing on  $[1/2, 1]$  and the unique value  $1/2 < \alpha(q) < 1$  where  $S_0(\alpha(q), \chi) = 0$  is given to 5 decimal places in the last column of Table 1 below. For fixed  $s > 1/2$ , we expect that all sufficiently large  $q$  should be nonexceptional in view of the factor  $\frac{1}{q^{1/2-s}}$  in (2.6). Even for the worst case  $s = 1/2$ , the first exceptional  $q$  occurs at  $q = 13340$  and there are only 218 exceptional  $q \leq 1,000,000$  and among these  $L_1(1/2, \chi) > 0$  for 174 of them. Up to one million, the largest least  $t$  required for  $L_t(s, \chi)$  to become positive is 8 for  $q = 925,097$ . Table 1 in Section 5 below contains a list of all exceptional  $q \leq 200,000$  at 0.5 and the smallest  $t$  value in each case.

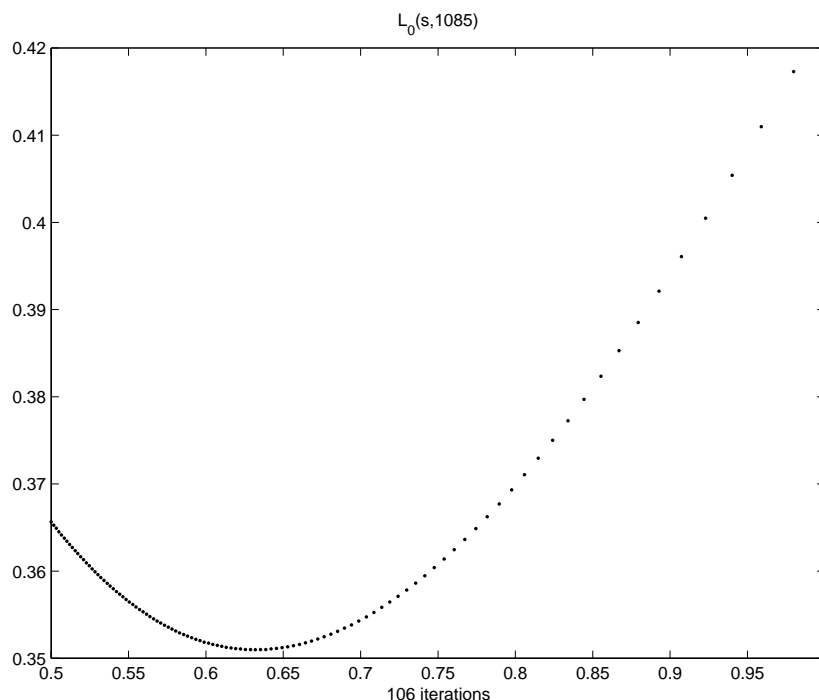
**2.2. A method for verifying  $L(s, \chi) > 0$  for  $0 < s < 1$ .** Theorem 2.1 gives us a way to prove that  $L(s, \chi) > 0$  at a particular point  $s$  by evaluating an exact finite sum. However the following simple observation allows us to extend it to a numerical method for verifying that  $L(s, \chi) > 0$  in an interval. By the functional equation [4], it suffices for us to check this for  $1/2 \leq s \leq 1$  for us to deduce that it has no real zero.

**Lemma 2.3.** *Let  $f(s) \in C^1[a, b]$  and assume that  $|f'(s)| \leq g(s)$  for  $s \in [a, b]$  and a function  $g(s)$  which is positive and decreasing on  $[a, b]$ . Then from  $f(s_0) > 0$  for some  $s_0 \in (a, b)$ , we can deduce  $f(s) > 0$  for  $s \in [s_0, s_0 + \frac{f(s_0)}{g(s_0)}]$ .*

*Proof.* Clearly we may assume  $f(s) \leq f(s_0)$ . We then have

$$f(s_0) - f(s) \leq \int_{s_0}^s |f'(t)| dt \leq \int_{s_0}^s g(t) dt \leq g(s_0)(s - s_0).$$

So we have  $f(s) \geq f(s_0) - g(s_0)(s - s_0) > 0$  for  $s_0 \leq s < s_0 + \frac{f(s_0)}{g(s_0)}$ . □

FIGURE 1.  $q=1085$ .

We may apply Lemma 2.3 to  $f(s) = L_t(s, \chi)$  since

$$|L'_t(s, \chi)| \leq \sum_{(n,q)=1, n=2}^{(t+1)q-1} \frac{\log n}{n^s} := g(s)$$

is clearly decreasing. We start with  $s_0 = 1/2$  and pick a  $t$  (for example the least  $t$ ) such that  $L_t(1/2, \chi) > 0$ . Such a  $t$  must exist if  $L(1/2, \chi) > 0$  which in turn is widely believed to be true and K. Soundararajan [12] has shown that at least  $7/8$  of the quadratic fields have  $L(1/2, \chi) \neq 0$ . Computationally, M. Rubinstein [8] has computed  $L(1/2, \chi)$  for  $q$  up to 100,000,000 to 15 decimal places, and they are all positive.

We then iteratively define the new point  $s_{i+1} := s_i + L_t(s_i, \chi)/g(s_i)$  and check the positivity of  $L_t(s_{i+1}, \chi)$ . When  $s_{i+1} \geq 1$ , we have verified the nonexistence of a real zero. In practice, we allow a small positive tolerance  $\epsilon > 0$  and the algorithm pseudocode is given below.

**ALGO 1**

**Find a  $t$  such that  $L_t(1/2, \chi) > \epsilon$  and set  $s = 1/2$ ;**

**while ( $s < 1$  and  $L_t(s, \chi) > \epsilon$ ) do**

$$s = s + L_t(s, \chi) / \sum_{(n,q)=1, n=2}^{(t+1)q-1} \frac{\log n}{n^s};$$

**if  $s > 1$  then NO POSITIVE REAL ZERO**

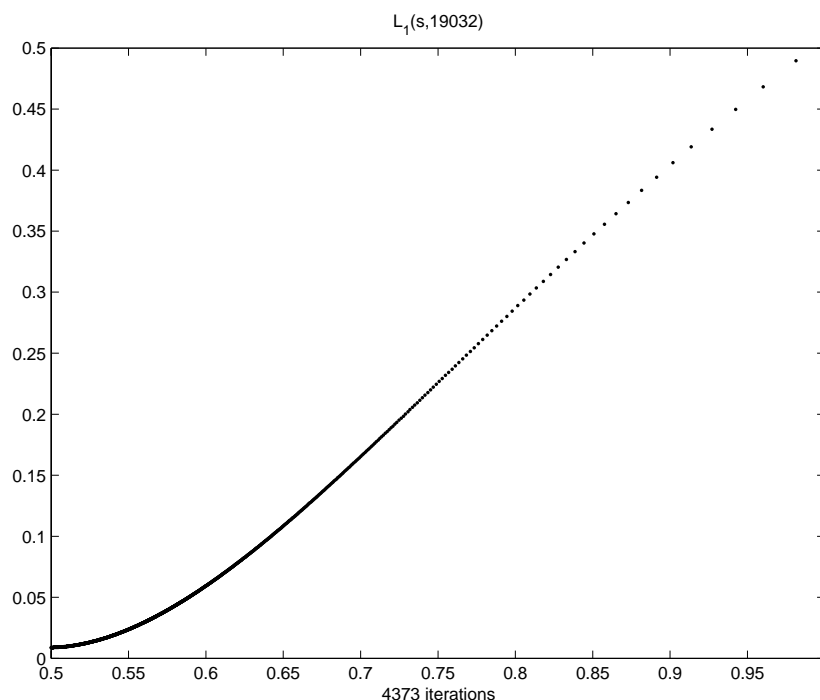


FIGURE 2.  $q=19032$ .

In this way we obtain Theorem 1.1. The progress of the algorithms is best illustrated in the plots of  $L_0(s, \chi)$  for  $q = 1085$  requiring 106 iterations in Figure 1 and  $L_1(s, \chi)$  for  $q = 19032$  in Figure 2 requiring 4373 iterations for  $\epsilon = 10^{-5}$ . The  $t$  values used are the least with  $L_t(1/2, \chi) > 0$ . These are the simplest cases. More iterations are needed usually (see Table 1). More details of the numerical computations will be given in Section 5.

ALGO 1 has the defect that the program will fail if we encounter an  $s$  with  $1/2 < s < 1$  and  $L_t(s, \chi) < \epsilon$  though  $L_t(s, \chi)$  may be positive throughout (this does not occur in the range of  $q$  that we computed above). One way to get around this is to note that the condition “ $L_t(s, \chi) \geq 0 \Rightarrow L(s, \chi) > 0$ ” is pointwise so that we may choose different  $t$  at different  $s$ . The obvious thing to do is to pick the least  $t$  such that  $L_t(s, \chi) > \epsilon$  for each  $s$ , which incurs no additional computational cost at each point evaluation since  $L_t(s, \chi)$  is computed as  $L_t(s, \chi) = L_{t-1}(s, \chi) + S_t(s, \chi)$  but we found experimentally that the pointwise computational saving is far outweighed by the larger number of iterations needed for using smaller  $t$ . The program will now work whenever  $L(s, \chi) > \epsilon$  throughout  $[1/2, 1]$  but it may still be necessary to pick a sufficiently small  $\epsilon$ . However if we set  $\alpha_t(s)$  to be the right-hand side of (2.6) and pick for each  $s$  the least  $t$  such that  $L_t(s, \chi) > \alpha_t(s)$ , the program is guaranteed to succeed as long as  $L(s, \chi) > 0$  in  $[1/2, 1]$ . Note that such a  $t$  must exist if  $L(s, \chi) > 0$  since  $\alpha_t(s) \rightarrow 0$  in  $t$  and  $L_t(s, \chi)$  is eventually positive. It also has the advantage of ensuring that  $L_t(s, \chi) > L(s, \chi)/2$  so that it is more efficient because the number of iterations is much less than picking the least  $t$  making  $L_t(s, \chi) > 0$ . However the value of  $t$  chosen will be 0 most of the time, and we find experimentally

that the naive ALGO 1 with a fixed  $t$  greater than the minimum necessary actually performed better.

### 3. PROOF OF MAIN RESULTS

**3.1. A Fourier expansion.** In this section, we will prove our main estimates in Theorems 2.1 and 2.2 essentially following Davenport's argument extended to  $s < 1$ . We consider for any real  $s > 0$  and  $\nu = 1, 2, 3, \dots$  the expansion of

$$f(x) = \frac{1}{(\nu + x)^s} \sim \frac{a_0}{2} + \sum_{m=1}^{\infty} (a_m \cos 2\pi mx + b_m \sin 2\pi mx), \quad 0 < x < 1,$$

in a Fourier series of period 1.

The coefficients are

$$(3.1) \quad a_m = 2 \int_0^1 \frac{\cos 2\pi mx}{(\nu + x)^s} dx, \quad b_m = 2 \int_0^1 \frac{\sin 2\pi mx}{(\nu + x)^s} dx.$$

Integrating (3.1) by parts gives for each  $k \geq 2$ ,

$$(3.2) \quad a_m = \sum_{j=1}^k (-1)^{j-1} \frac{F_{2j}}{m^{2j}} + (-1)^k \frac{2s(s+1) \cdots (s+2k-1)}{(2\pi m)^{2k}} \int_0^1 \frac{\cos 2\pi mx}{(\nu + x)^{s+2k}} dx,$$

(3.3)

$$b_m = \sum_{j=1}^k (-1)^{j-1} \frac{F_{2j-1}}{m^{2j-1}} + (-1)^k \frac{2s(s+1) \cdots (s+2k-2)}{(2\pi m)^{2k-1}} \int_0^1 \frac{\sin 2\pi mx}{(\nu + x)^{s+2k-1}} dx,$$

where

$$(3.4) \quad F_1 = \frac{1}{\pi} \left\{ \frac{1}{\nu^s} - \frac{1}{(\nu+1)^s} \right\},$$

$$(3.5) \quad F_j = \frac{2s(s+1) \cdots (s+j-2)}{(2\pi)^j} \left\{ \frac{1}{\nu^{s+j-1}} - \frac{1}{(\nu+1)^{s+j-1}} \right\}, \quad j \geq 2.$$

**Lemma 3.1.** For  $k \geq 2$ , we have

$$(3.6) \quad a_m = \sum_{j=1}^{k-1} (-1)^{j-1} \frac{F_{2j}}{m^{2j}} + (-1)^{k-1} \theta_{m,k} \frac{F_{2k}}{m^{2k}},$$

$$(3.7) \quad b_m = \sum_{j=1}^{k-1} (-1)^{j-1} \frac{F_{2j-1}}{m^{2j-1}} + (-1)^{k-1} \phi_{m,k} \frac{F_{2k-1}}{m^{2k-1}},$$

where  $0 < \theta_{m,k} < 1$ ,  $0 < \phi_{m,k} < 1$ .

*Proof.* Since clearly we have

$$\begin{aligned} 0 < I_{m,2k} &:= \int_0^1 \frac{\cos 2\pi mx}{(\nu + x)^{s+2k}} \\ &< \int_0^1 \frac{dx}{(\nu + x)^{s+2k}} = \frac{1}{s+2k-1} \left\{ \frac{1}{\nu^{s+2k-1}} - \frac{1}{(\nu+1)^{s+2k-1}} \right\}, \end{aligned}$$

we may write  $I_{m,2k} = \frac{1-\theta_{m,k}}{s+2k-1} \left\{ \frac{1}{\nu^{s+2k-1}} - \frac{1}{(\nu+1)^{s+2k-1}} \right\}$  for some  $\theta_{m,k} \in (0, 1)$ . Equation (3.6) follows from (3.2).  $\square$

**3.2. Proof of Theorem 2.2 for arbitrary primitive character.** We first derive general estimates which hold for any primitive character  $\chi$  (not necessary real or even) which may be of some independent interest. First we have (see [4, p. 68])

$$(3.8) \quad \tau_m(\chi) = \sum_{n=1}^{q-1} \chi(n)e^{2\pi imn/q} = \bar{\chi}(m)\tau(\chi),$$

where the Gauss sum  $\tau(\chi) := \tau_1(\chi)$  satisfies  $\tau(\chi)\tau(\bar{\chi}) = \chi(-1)q$ . It follows that

$$(3.9) \quad \sum_{n=1}^{q-1} \chi(n) \cos 2\pi mn/q = \bar{\chi}(m)\tau(\chi), \quad \sum_{n=1}^{q-1} \chi(n) \sin 2\pi mn/q = 0$$

if  $\chi$  is even, and

$$(3.10) \quad \sum_{n=1}^{q-1} \chi(n) \cos 2\pi mn/q = 0, \quad \sum_{n=1}^{q-1} \chi(n) \sin 2\pi mn/q = -i\bar{\chi}(m)\tau(\chi)$$

if  $\chi$  is odd, and we have

**Lemma 3.2.** For  $k \geq 2, s > 0$ , and any primitive Dirichlet character,

$$(3.11) \quad \frac{q^s S_\nu(s, \chi)}{\tau(\chi)} = \sum_{j=1}^{k-1} (-1)^{j-1} F_{2j} L(2j, \bar{\chi}) + \theta_k F_{2k} \zeta(2k), \quad \chi \text{ even},$$

$$(3.12) \quad \frac{q^s S_\nu(s, \chi)}{-i\tau(\chi)} = \sum_{j=1}^{k-1} (-1)^{j-1} F_{2j-1} L(2j-1, \bar{\chi}) + \phi_k F_{2k-1} \zeta(2k-1), \quad \chi \text{ odd},$$

where  $|\theta_k| < 1$  and  $|\phi_k| < 1$ .

*Proof.* For  $\chi$  even, we have by the Fourier expansion of  $f$  and (3.9),

$$S_\nu(s, \chi) = \sum_{n=1}^{q-1} \frac{\chi(n)}{(q\nu+n)^s} = \frac{1}{q^s} \sum_{n=1}^{q-1} \chi(n) f\left(\frac{n}{q}\right) = \frac{\tau(\chi)}{q^s} \sum_{m=1}^{\infty} a_m \bar{\chi}(m),$$

and (3.11) follows from summing (3.6) with  $\theta_k = \sum \frac{(-1)^{k-1} \theta_{m,k} \bar{\chi}(m)}{m^{2k}} / \zeta(2k)$  which has the obvious bound. The odd case is similar.  $\square$

*Proof of Theorem 2.2.* Choosing  $k = 2$  and summing over (3.11) for  $\nu = t + 1$  to  $\infty$  using (3.5) gives

$$(3.13) \quad E_{t+1}(s, \chi) = \frac{\tau(\chi)}{q^s} \left( \frac{s}{2\pi^2} \frac{L(2, \bar{\chi})}{(t+1)^{s+1}} + \theta_2 \frac{s(s+1)(s+2)}{8\pi^4} \frac{\zeta(4)}{(t+1)^{s+3}} \right).$$

We now use the trivial bound  $|L(2, \bar{\chi})| \leq \zeta(2) = \frac{\pi^2}{6}$ ,  $\zeta(4) = \frac{\pi^4}{90}$  and the fact that  $|\tau(\chi)| = \sqrt{q}$  in (3.13) to obtain (2.6). A similar estimate gives (2.7) in the odd case.  $\square$

We also need the following

**Lemma 3.3.** For  $\nu > 5/4$  and  $s \geq 3/2$ , it holds that

$$(3.14) \quad \frac{1}{\nu^s} - \frac{1}{(\nu+1)^s} > \frac{1}{\nu^{s+2}} - \frac{1}{(\nu+1)^{s+2}}.$$

*Proof.* Since  $\nu > 1$ , by multiplying both sides of (3.14) by  $\nu^{s+2}(\nu + 1)^{s+2}$ , we see that it holds if and only if  $(\nu + 1)^{s+3}(\nu - 1) > \nu^{s+3}(\nu + 2)$  and clearly this will be true for all  $s \geq 3/2$  if it is true at  $s = 3/2$ . We need to prove that

$$\left(\frac{\nu + 1}{\nu}\right)^{9/2} > \frac{\nu + 2}{\nu - 1}$$

or equivalently  $f(x) = (2 - x)x^{9/2} - (2x - 1) > 0$ , for  $x = (\nu + 1)/\nu \in (1, 9/5)$ , or that the polynomial  $h(y) = f(y^2) = -y^{11} + 2y^9 - 2y^2 + 1$  is positive for  $y = \sqrt{x} \in (1, 3/\sqrt{5})$  and this is true since it is easily shown that  $h(1) = 0, h'(1) = 3 > 0$  and the only positive roots of  $h$  greater than 1 is around  $1.35 > 3/\sqrt{5}$ .  $\square$

**Lemma 3.4.** *For any real nonprincipal character  $\chi$ ,  $L(2, \chi) > \frac{\pi^2}{15}$ .*

*Proof.*

$$(3.15) \quad L(2, \chi) = \prod_{p \geq 2} (1 - \chi(p)/p^2)^{-1} > \prod_{p \geq 2} (1 + 1/p^2)^{-1} = \zeta(4)/\zeta(2) = \pi^2/15.$$

$\square$

**3.3. Proof of Theorem 2.1 for even real primitive characters.** We now assume  $\chi$  is real primitive and even. In this case Gauss determined the sign of the Gauss sum so that  $\tau(\chi) = \sqrt{q}$ . For  $1/2 \leq s \leq 1$ , we pick  $k = 2$  in (3.11) and use  $\zeta(4) = \pi^4/90$  and (3.15) to obtain

$$\frac{S_\nu(s, q)q^s}{\sqrt{q}s} > \frac{1}{30} \left( \frac{1}{\nu^{s+1}} - \frac{1}{(\nu + 1)^{s+1}} \right) - \frac{1}{120} \left( \frac{1}{\nu^{s+3}} - \frac{1}{(\nu + 1)^{s+3}} \right),$$

and this gives (2.3) by setting  $\nu = 1$ . Inequality (2.4) follows from Lemma 3.3.  $\square$

#### 4. ESTIMATES FOR SHIFTED CYCLE SUMS

**4.1. Extension of a result of Leu and Li.** In 1996, Leu and Li [5] generalized Davenport’s result on  $S_\nu(1, \chi)$  to shifted cycle sums. We shall now extend this to  $1/2 \leq s \leq 1$ . The main ideas are essentially those of Davenport but the details are more involved. Throughout this section, we assume  $\chi$  is real, primitive and even. We define for  $s > 0$  and  $\nu = 0, 1, 2, 3, \dots$

$$(4.1) \quad A_\nu(s, \chi) := \sum_{n=\nu q+1}^{\nu q+\lfloor q/2 \rfloor} \frac{\chi(n)}{n^s}, \quad B_\nu(s, \chi) := \sum_{n=\nu q+\lfloor q/2 \rfloor+1}^{(\nu+1)q-1} \frac{\chi(n)}{n^s},$$

$$(4.2) \quad T_\nu(s, \chi) := B_\nu(s, \chi) + A_{\nu+1}(s, \chi) = \sum_{n=\nu q+\lfloor q/2 \rfloor+1}^{(\nu+1)q+\lfloor q/2 \rfloor} \frac{\chi(n)}{n^s}.$$

Note that  $S_\nu(s, \chi) = A_\nu(s, \chi) + B_\nu(s, \chi)$ . The main estimate is the following generalization of Leu and Li’s extension of Davenport’s result to shifted sum:

**Theorem 4.1.** *If  $\chi$  is real, even and primitive,  $\nu = 0, 1, 2, \dots, 1/2 \leq s \leq 1$ , then*

$$(4.3) \quad T_\nu(s, \chi) < 0.$$

*Furthermore, for  $\nu \geq 1$  we have more explicitly*

$$(4.4) \quad T_\nu(s, \chi) < \frac{s}{q^{s-1/2}} c(s) \left\{ \frac{1}{(\nu + 1/2)^{s+1}} - \frac{1}{(\nu + 3/2)^{s+1}} \right\},$$

where

$$c(s) = \frac{(s+1)(s+2)}{720} - \frac{1}{32} < -\frac{11}{480}.$$

The following corollary generalizing that in [5] is immediate.

**Corollary 4.2.** *We have for any  $t_1, t_2 \geq 0$ , and  $1/2 \leq s \leq 1$ ,*

$$(4.5) \quad \sum_{\nu=0}^{t_1} S_\nu(s, \chi) < L(s, \chi) < A_0(s, \chi) + \sum_{\nu=0}^{t_2} T_\nu(s, \chi),$$

$$(4.6) \quad A_\nu(s, \chi) > 0 \text{ for } \nu \geq 1, \quad A_0(s, \chi) > L(s, \chi), \quad B_\nu(s, \chi) < 0, \text{ for } \nu \geq 0.$$

We will need the following

**Lemma 4.3.** *For any real nonprincipal character  $\chi$ , we have*

$$(4.7) \quad H(\chi) := \sum_{m \geq 1} \frac{(-1)^m \chi(m)}{m^2} < \begin{cases} -\frac{\pi^2}{12} & \text{if } \chi(2) \in \{0, -1\}, \\ -\frac{\pi^2}{16} & \text{if } \chi(2) = 1. \end{cases}$$

*Proof.* We have

$$H(\chi) = \left(-1 + \frac{\chi(2)}{2^2}\right) \sum_{m \text{ odd}} \frac{\chi(m)}{m^2} = -\left(1 - \frac{\chi(2)}{2^2}\right) \prod_{p \geq 3} \left(1 - \frac{\chi(p)}{p^2}\right)^{-1},$$

and the result follows from

$$\prod_{p \geq 3} \left(1 - \frac{\chi(p)}{p^2}\right)^{-1} \geq \prod_{p \geq 3} \left(1 + \frac{1}{p^2}\right)^{-1} = \left(1 + \frac{1}{2^2}\right) \frac{\zeta(4)}{\zeta(2)} = \frac{\pi^2}{12}.$$

□

**4.2. Proof of Theorem 4.1.** We consider now the Fourier expansion of

$$(4.8) \quad f(x) = \frac{1}{(\nu+x)^s} \sim \frac{a'_0}{2} + \sum_{m=1}^{\infty} (a'_m \cos 2\pi mx + b'_m \sin 2\pi mx), \quad 1/2 < x < 3/2,$$

Since  $a'_m = 2 \int_{1/2}^{3/2} \frac{\cos 2\pi mx}{(\nu+x)^s} dx$ , we have as in (3.6) with  $k = 2$ ,

$$(4.9) \quad a'_m = (-1)^m \frac{2s}{(2\pi m)^2} \left\{ \frac{1}{(\nu+1/2)^{s+1}} - \frac{1}{(\nu+3/2)^{s+1}} \right\} \\ + (-1)^{m+1} \frac{2s(s+1)(s+2)}{(2\pi m)^4} \left\{ \frac{1}{(\nu+1/2)^{s+3}} - \frac{1}{(\nu+3/2)^{s+3}} \right\} \\ + \frac{2s(s+1)(s+2)(s+3)}{(2\pi m)^4} \int_{1/2}^{3/2} \frac{\cos 2\pi mx}{(\nu+x)^{s+4}} dx.$$

Since the amplitude in the last integral is decreasing, its sign must be that of  $\cos 2m(1/2)\pi = (-1)^m$ . The mean value theorem gives

$$(4.10) \quad \int_{1/2}^{3/2} \frac{\cos 2\pi mx}{(\nu+x)^{s+4}} dx = (-1)^m \theta'_m \int_{1/2}^{3/2} \frac{1}{(\nu+x)^{s+4}} dx,$$

where  $0 < \theta'_m < 1$ . It follows that we have

$$(4.11) \quad a'_m = (-1)^m \frac{2s}{(2\pi m)^2} \left\{ \frac{1}{(\nu + 1/2)^{s+1}} - \frac{1}{(\nu + 3/2)^{s+1}} \right\} \\ + (-1)^{m+1} \frac{2s(s+1)(s+2)}{(2\pi m)^4} \left\{ \frac{1}{(\nu + 1/2)^{s+3}} - \frac{1}{(\nu + 3/2)^{s+3}} \right\} \theta'_{m,2},$$

where  $0 < \theta'_{m,2} = 1 - \theta'_m < 1$  depends on both  $\nu$  and  $s$ .

By the Gauss sum (3.9), we get

$$(4.12) \quad \frac{q^s T_\nu(s, \chi)}{\sqrt{q}} = \frac{s}{2\pi^2} \left\{ \frac{1}{(\nu + 1/2)^{s+1}} - \frac{1}{(\nu + 3/2)^{s+1}} \right\} \sum_{m=1}^{\infty} \frac{(-1)^m \chi(m)}{m^2} \\ + \frac{s(s+1)(s+2)}{8\pi^4} \left\{ \frac{1}{(\nu + 1/2)^{s+3}} - \frac{1}{(\nu + 3/2)^{s+3}} \right\} \sum_{m=1}^{\infty} \frac{(-1)^{m+1} \chi(m)}{m^4} \theta'_{m,2}(s).$$

If  $\nu \geq 1$ , the right-hand side can be bounded above using Lemma 4.3,

$$\left| \sum_{m=1}^{\infty} \frac{(-1)^{m+1} \chi(m)}{m^4} \theta'_{m,2}(s) \right| \leq \zeta(4) = \pi^4/90,$$

and Lemma 3.3 which yields (4.4).

For  $\nu = 0$ , we note that

$$(4.13) \quad \frac{q^{s-1/2} T_0(s, \chi)}{s} = \frac{1}{2\pi^2} \left( 2^{s+1} - \frac{2^{s+1}}{3^{s+1}} \right) \sum_{m=1}^{\infty} \frac{(-1)^m \chi(m)(m^2 - \lambda(s)\theta'_{m,2}(s))}{m^4},$$

where

$$(4.14) \quad \lambda(s) = \frac{(s+1)(s+2)}{9\pi^2} \left( \frac{3^{s+3} - 1}{3^{s+1} - 1} \right).$$

It thus suffices for us to show that

$$(4.15) \quad Y(s) := \sum_{m=1}^{\infty} \frac{(-1)^m \chi(m)(m^2 - \lambda(s)\theta'_{m,2}(s))}{m^4} < 0.$$

We need two more lemmas.

**Lemma 4.4.** For  $1/2 \leq s \leq 1$ , we have

$$(4.16) \quad 0.46044 \dots = \frac{5(27\sqrt{3} - 1)}{12\pi^2(3\sqrt{3} - 1)} = \lambda(1/2) \leq \lambda(s) \leq \lambda(1) = \frac{20}{3\pi^2} = 0.67547 \dots$$

*Proof.* We set  $s = S - 1$  and  $\mu(S) = S(S + 1)(9 \cdot 3^S - 1)/(3^S - 1) = 9\pi^2\lambda(s)$ , and we observe that  $\mu'(S)$  has the same sign as

$$f(S) = (2S + 1)(9 \cdot 3^S - 1)(3^S - 1) - 8S(S + 1)3^S \log 3.$$

Since  $3^S - 1 = e^{S \log 3} - 1 \geq S \log 3$ , we have

$$f(S) \geq (S \log 3)((10S + 1)3^S - (2S + 1)) \\ \geq (S \log 3)((10S + 1) - (2S + 1)) \geq 8S^2 \log 3 \geq 0$$

for  $S \geq 0$ . Hence  $\lambda(s)$  increases with  $s \geq -1$  and the results follow. □

As in [5] we will need to estimate  $\theta'_{1,2}$ . From (4.10) with  $\nu = 0, m = 1$ , we have

$$\theta'_{1,2}(s) = 1 + \frac{s + 3}{\left(2^{s+3} - \frac{2^{s+3}}{3^{s+3}}\right)} \int_{1/2}^{3/2} \frac{\cos 2\pi x}{x^{s+4}} dx$$

so that integrating by parts three times gives

$$(4.17) \quad \lambda(s)\theta'_{1,2}(s) = 1 - \frac{\pi 3^{s+1}}{2^s(3^{s+1} + 1)} I(s),$$

where

$$(4.18) \quad I(s) = \int_{1/2}^{3/2} \frac{-\sin 2\pi x}{x^{s+1}} dx.$$

**Lemma 4.5.** *For  $1/2 \leq s \leq 1$ , we have*

$$(4.19) \quad \lambda(s)\theta'_{1,2}(s) \leq 1 - \frac{9\pi}{16} \int_{1/2}^{3/2} \frac{-\sin 2\pi x}{x^{3/2}} dx = 0.50590 \dots$$

*Proof.* We split the integral into two parts and set  $x = 2 - x$  in  $\int_1^{3/2}$  to obtain

$$I(s) = \int_{1/2}^1 -\sin(2\pi x) f(s, x) dx \quad \text{with} \quad f(s, x) = \frac{1}{x^{s+1}} - \frac{1}{(2-x)^{s+1}}.$$

Since  $x \leq 2 - x$  for  $x \leq 1$  and the function  $g(x) = \frac{\log x}{x^{s+1}}$  is increasing for  $s \geq -1, x \leq 1$ , the integrand in  $I'(s)$  is nonnegative and hence  $I(s)$  is increasing. Since  $\frac{\pi 3^{s+1}}{2^s(3^{s+1}-1)}$  decreases for  $s > -1$ , the result follows. □

We are now ready to prove (4.15). Assume first (the easy case) where  $\chi(2) \in \{0, -1\}$ . From the definition of  $Y(s)$  in (4.15), (4.7) and Lemma 4.4 we have

$$Y(s) < -\frac{\pi^2}{12} + \lambda(s)\zeta(4) \leq -\frac{\pi^2}{12} + \frac{20}{3\pi^2} \frac{\pi^4}{90} = \frac{-\pi^2}{108} < 0.$$

If  $\chi(2) = 1$ , we consider the first three terms in (4.15)

$$(4.20) \quad Y(s) = H(\chi) + \lambda(s)\theta'_{1,2}(s) - \lambda(s)\frac{\theta'_{2,2}(s)}{16} - \lambda(s) \sum_{m \geq 3} \frac{(-1)^m \chi(m)\theta'_{m,2}(s)}{m^4},$$

and using (4.7), the fact that  $\chi(2) > 0, \lambda(s) > 0, 0 < \theta'_{i,2}(s) < 1$  and a trivial bound in the last term give

$$(4.21) \quad \begin{aligned} Y(s) &< -\frac{\pi^2}{16} + \lambda(s)\theta'_{1,2}(s) + \lambda(s) \sum_{m \geq 3} \frac{1}{m^4} \\ &\leq -\frac{\pi^2}{16} + 1 - \frac{9\pi}{16} \int_{1/2}^{3/2} \frac{\sin 2\pi x}{x^{3/2}} dx + \frac{20}{3\pi^2} \left( \frac{\pi^4}{90} - \frac{17}{16} \right) \\ &\approx -0.0975579 \dots < 0, \end{aligned}$$

where we used Lemma 4.5 in the last inequality. This completes the proof of Theorem 4.1.

## 5. NUMERICAL RESULTS

We applied ALGO 1 to primitive even real characters of conductor  $q$  up to 200,000 choosing the smallest  $t$  for which  $L_t(1/2, \chi) > 0$  and using  $\epsilon = 0.00001$ . It is found that the program always terminates with  $s > 1$  after finitely many steps and this proves Theorem 1.1. The computations for two simple cases  $q = 1085$  and 19032 are given in Figure 1 and Figure 2 where each plotted point corresponds to one iteration (one function and one derivative evaluation). The computations usually require a large number of iterations and take a long time to run. Statistics for the computations for the 46 exceptional primitive conductors  $q$  up to 200,000 for which  $S_0(s, \chi) < 0$  is summarised in Table 1. Each row gives the conductor  $q$ , the class number  $h(q)$  of  $Q(\sqrt{q})$ , its regulator  $R$ , the negative values of  $S_0(1/2, \chi)$ , the smallest  $t$  for which  $L_t(1/2, \chi) > 0$ , the value of  $L_t(s, \chi)$ , the number of iterations, the clock time needed in seconds and finally the unique value  $1/2 < \alpha(q) < 1$  where  $S_0(s, \chi)$  crosses the zero line. The reader should be able to verify these computations independently by checking the number of iterations used. The timing of course depends on too many factors and is only meant as a guide of the relative amount of time needed. We have also proved numerically that  $S'_0(s, \chi) > 0$  for the exceptional  $q$  values at  $1/2$  in Table 1 using Lemma 2.3 with  $f(s) = S'_0(s, \chi)$  and  $g(s) = \sum_{(n,q)=1, n=2}^{(t+1)q-1} \frac{(\log n)^2}{n^s}$  and a similar algorithm to ALGO 1. The computations can be done relatively fast as compared to the positivity of  $L(s, \chi)$  because  $S'_0(s, \chi)$  is bounded further from zero because of the additional  $\log n$  term. The value of  $\alpha(q)$  is then determined by simple bisection.

We note that  $S_0(1/2, \chi) < 0$  tends to occur only for small class numbers though we have yet to formalise an exact relationship. The most time consuming case occurs for  $q = 142,637$  which requires 776,099 iterations over more than 5 days (469,354 seconds) to run on our system. This is because  $L_t(1/2, \chi) = 0.00001$  is exceptionally small. We note that we can usually improve the performance by choosing a bigger  $t$  than the least one which makes  $L_t(1/2, \chi) > 0$ . For  $q = 142,637$ , choosing  $t = 3$  in ALGO 1 requires only 121,254 iterations and runs more than 5 times faster (90175 seconds). Note that in this case,  $L_3(0.5, \chi) \approx 0.00378$  is much closer to  $L(0.5, \chi) \approx 0.00591$ . It is clear we can always do better by choosing  $t$  so that  $L_t(0.5, \chi) > \alpha L(0.5, \chi)$  for some  $\alpha > 0.5$ . Note that this can be done without computing  $L(s, \chi)$  using (2.6).

The algorithms are programmed in C with independent verification using PARI-GP. The computations are done on a Linux PC cluster which comprises 8 500-MHz Pentium III PC with 256M RAM and total disk space of 8 GB, in the Department of Mathematics at the National University of Singapore. We applied the usual computational tricks. For example, since ALGO 1 is applied for a fixed  $q$  at many different  $s$ , the values of  $\log n$  are precomputed in double precision in a table and values of  $n$  for which  $\chi(n)$  is  $\pm 1$  are remembered as indices. This is done only once and is then used at all the points where the function is evaluated. Note also that in most cases (e.g., when  $Z/q^*$  is cyclic),  $\chi(n) = 1$  exactly for the quadratic residues which are found easily by taking squares up to  $\lfloor q/2 \rfloor$  and using  $\chi(n) = \chi(-n)$  without the need for the Euclidean algorithm for the Kronecker symbol.

TABLE 1. Exceptional  $q$  at  $1/2$  up to 200,000: Time and iterations needed

$q$	$h(q)$	$R$	$S_0(0.5, \chi)$	$t$	$L_t(0.5, \chi)$	Iterations	Time (sec)	$\alpha(q)$
13340	4	6.1355	-0.01645	3	0.00089	27509	1695	0.54909
14693	1	18.001	-0.01389	4	0.00025	179259	50523	0.55400
16557	1	25.291	-0.00912	1	0.00194	23269	2845	0.53545
19032	4	8.7555	-0.00477	1	0.00881	4373	61	0.51984
37901	1	35.072	-0.01105	2	0.00208	71866	8738	0.53937
42573	6	6.4281	-0.00975	1	0.00101	52572	3185	0.53544
50648	2	24.956	-0.00830	1	0.00398	18831	5057	0.52860
50853	4	11.211	-0.00012	1	0.01072	13639	4266	0.50106
53633	3	27.754	-0.00382	1	0.01260	17585	9411	0.51296
55037	5	7.0673	-0.00861	1	0.00100	103674	60555	0.53643
55733	1	32.339	-0.00442	1	0.00503	46636	5712	0.52492
60357	4	10.807	-0.01284	2	0.00070	97518	11687	0.54249
61333	1	63.313	-0.00537	1	0.00683	31074	4227	0.51987
61817	3	32.109	-0.00507	1	0.01165	16448	5334	0.51494
63416	1	71.246	-0.00921	1	0.00407	2029	3047	0.52620
68317	4	18.350	-0.00168	1	0.01088	23487	5633	0.50844
70949	1	58.183	-0.00635	1	0.00441	46042	8621	0.52398
89448	2	46.142	-0.00257	1	0.01150	8607	1269	0.51049
90461	1	62.809	-0.01184	2	0.00161	105042	35418	0.53535
91352	2	38.874	-0.00351	1	0.00917	15236	8288	0.51441
95717	1	38.805	-0.00164	1	0.00772	50499	65342	0.51218
96413	1	57.394	-0.00035	1	0.00968	36022	35372	0.50288
106917	6	10.481	-0.00756	1	0.00316	48543	44436	0.52789
109133	1	44.016	-0.00482	1	0.00460	71691	15545	0.52577
123653	1	52.612	-0.00120	1	0.00835	50364	12393	0.50866
125877	1	69.864	-0.01420	3	0.00078	180915	264353	0.54003
134357	4	13.180	-0.00774	1	0.00179	121471	168781	0.53316
137805	2	39.716	-0.00966	1	0.00146	137805	66540	0.53007
140460	4	30.441	-0.00670	1	0.00758	10912	6151	0.51879
142637*	5	11.667	-0.00960	1	0.00001	776099*	469354*	0.53604
144905	4	40.588	-0.01391	1	0.00321	46556	71570	0.52510
145517	3	23.139	-0.00751	1	0.00248	100927	163109	0.52807
147453	6	12.188	-0.00605	1	0.00469	44888	38787	0.52391
147773	3	16.689	-0.00418	1	0.00523	79303	84223	0.52329
159437	5	12.646	-0.00297	1	0.00664	64293	77721	0.51627
161192	2	46.526	-0.00065	1	0.01163	19745	23023	0.50402
161229	12	8.7033	-0.01282	2	0.00207	86219	146494	0.53141
170813	1	58.682	-0.00187	1	0.00765	65035	95385	0.51228
174605	6	14.352	-0.00213	1	0.00823	41175	51431	0.51120
176657	4	39.192	-0.00613	1	0.01030	33230	48035	0.51607
178485	4	22.371	-0.00699	1	0.00412	41678	47460	0.52435
179837	4	17.079	-0.00079	1	0.00897	46694	103994	0.50582
180197	1	66.343	-0.00293	1	0.00663	68718	119778	0.51614
192488	2	58.079	-0.01242	1	0.00028	137823	128591	0.53013
193973	4	14.228	-0.00254	1	0.00687	70282	120195	0.51606
199132	1	158.85	-0.01131	1	0.00399	33981	48548	0.52414

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