On the Asymptotic Analysis of the Discrete Dirac Equation

Mattias Holschneider and Charles Gunn

SFB 288, Technical University Berlin *

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Abstract

We describe a discrete version of the one-dimensional Dirac equation. Images from computer simulations of this system led to our attempt to understand the asymptotic behavior. Using techniques of Fourier analysis and asymptotic analysis, we obtain results generally valid for operators on $L^2(\mathbf{Z})$ which commute with translation by two, which allow us to prove in the Dirac case that the critical angle β satisfies $\sin(\beta) \leq \tan(\mu)$, where μ is the discrete analog of mass, with strong evidence of equality.

1 Discrete 1D Dirac Equation

Consider the following discretization of the one-dimensional Dirac equation.

Recall the continuous Dirac equation for two spinors $\Phi = \Phi(u, v)$ and $\Psi = \Psi(u, v)$:

$$\begin{pmatrix} 0 & \partial_v \\ \partial_u & 0 \end{pmatrix} \begin{pmatrix} \Phi \\ \Psi \end{pmatrix} = i\, m \begin{pmatrix} \Phi \\ \Psi \end{pmatrix} \tag{1}$$

where $i = \sqrt{-1}$ and m is the mass of the electron, and (u, v) are *light-cone* coordinates, defined by:

$$(x, t) = \frac{1}{\sqrt{2}} \begin{pmatrix} u - v \\ u + v \end{pmatrix} \tag{2}$$

We make the domain discrete but leave the range continuous. Then the function values Φ, Ψ are defined on the midpoints of the edges of the diamond lattice depicted in Figure 1. We define a dynamical system on this lattice which we claim is a discrete version of (1). This dynamical system evolves from an initial *zigzag* configuration at time $t = 0$ according to the local interaction (see Figure 2):

$$\begin{pmatrix} \Phi_{t+1} \\ \Psi_{t+1} \end{pmatrix} = \mathbf{U} \begin{pmatrix} \Psi_t \\ \Phi_t \end{pmatrix}, \quad \mathbf{U} = \begin{pmatrix} \cos(\mu) & i\sin(\mu) \\ i\sin(\mu) & \cos(\mu) \end{pmatrix} \tag{3}$$

*Current address: Sonderforschungsbereich 288, MA 8-5, Technische Universität, Strasse des 17 Juni 136, 10623 Berlin, Germany, {hols,gunn}@sfb288.math.tu-berlin.de

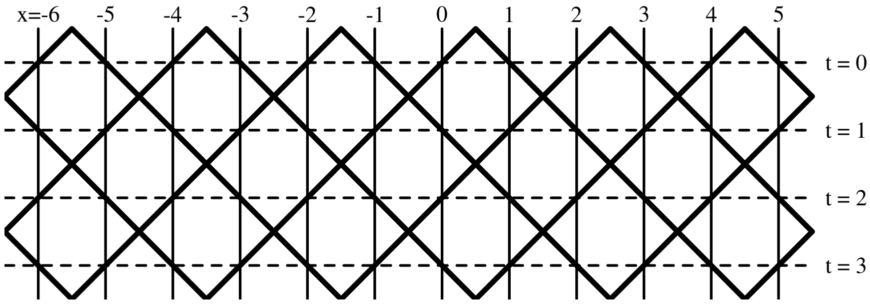

Figure 1: Φ and Ψ take values on midpoints of edges of the diamond lattice.

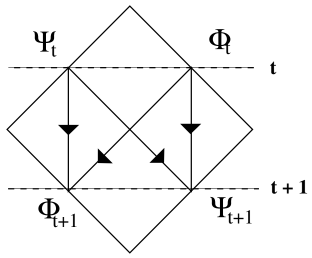

Figure 2: The discrete time evolution operates on adjacent pairs of sites.

1.1 Verification that this is a discrete version of the Dirac equation

To see that this system is a discrete version of the Dirac differential equation, define:

$$
\begin{aligned}
D_u\Phi &= \Phi_{t+1} - \Phi_t \\
M_v\Psi &= \frac{1}{2}(\Psi_{t+1} + \Psi_t)
\end{aligned}
$$

$$
\begin{aligned}
D_u\Phi &= (\cos(\mu) - 1)\Phi_t + i\sin(\mu)\Psi_t \\
&= -2\sin^2(\mu/2)\Phi_t + 2i\sin(\mu/2)\cos(\mu/2)\Psi_t & (4) \\
M_v\Psi &= \frac{1}{2}((\cos(\mu) + 1)\Psi_t + i\sin(\mu)\Phi_t) \\
&= \cos^2(\mu/2)\Psi_t + i\sin(\mu/2)\cos(\mu/2)\Phi_t & (5)
\end{aligned}
$$

Combining (4) and (5) yields:

$$D_u\Phi = -2i\tan(\mu/2)M_v\Psi \tag{6}$$

Setting $m = -2\tan(\mu/2)$ and letting the lattice step size go to zero, shows that this is a discrete version of the first half of (1); the second half can be similarly derived.

1.2 Definition of the evolution operator A

Closely related to this discrete dynamics is a discrete operator **A** constructed as follows. Let $x_{i,t}$ denote the value of the function Φ (or Ψ) at the i^{th} edge of the edge zigzag at time t. On even time steps, $x_{2i,t}$ is paired with $x_{2i+1,t}$ while on odd time steps, $x_{2i,t}$ is paired with its other neighbor, $x_{2i-1,t}$. (The exact nature of the pairing depends on whether the site $x_{0,0}$ lies on a / or a \ edge of the initial zigzag. Our discussion assumes the former, as shown in Figure 3).

Let $\mathbf{A}_e$ denote the operator on $L^2(\mathbf{Z})$ induced by the local evolution matrix $\mathbf{U}$. That is, the sequence $\{x_{i,t}\}$ is mapped to the sequence $\{x_{i,t+1}\}$ under $\mathbf{A}_e$ by the local action of $\mathbf{U}$ on the collection of paired sites. It is clear that $\mathbf{U} \in SU(2, C)$, so the induced $L^2(\mathbf{Z})$ operator $\mathbf{A}_e$ is norm-preserving and unitary. In addition, it commutes with translation by 2, that is, $[\mathbf{A}_e, T_2] = 0$, where T_k is right-translation by k. In the same way, let $\mathbf{A}_o$ denote the operator on odd time steps: $\mathbf{A}_o = T_1 \mathbf{A}_e T_1^*$. Define the composite operator $\mathbf{A}$ on $L^2(\mathbf{Z})$ by $\mathbf{A} = \mathbf{A}_o \mathbf{A}_e$. $\mathbf{A}$ gives the evolution after two time steps, one even and one odd (refer again to Figure 3). It is clear that iteration of $\mathbf{A}$ describes the evolution of the dynamical system described above. We first show some numerical results of the long-time behavior of this evolution.

1.3 Notation

Elements of $L^2(\mathbf{Z})$ will be denoted by small Roman letters, e.g., $s, t, ...$ The i^{th} entry of a sequence will be denoted by a subscript: s_i. Formally, $s = \{s_i\}$. We will make frequent use of the special sequence δ_k, defined by

$$\{\delta_k\}_i := \begin{cases} 1 & \text{if k = i} \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

1.4 Numerical simulation

We performed numerical simulation of this system with initial condition given by the sequence δ_0 and various values for μ. For $\mu = 0$ there is no propagation, i.e., $\mathbf{A}^n(\delta_0) = \delta_0$; for $\mu = \pi/2$ the initial pulse translates without diffusion along the right-hand light-cone, i.e., $\mathbf{A}^n(\delta_0) = \delta_{2n}$. (Note the factor of two, due to the fact that $\mathbf{A}$ represents 2 time steps of our original system.) For intermediate values the situation is more interesting. Figure 4 shows a typical evolution, for $\mu = \pi/8$. Intensity values are inversely proportional to the amplitude of the complex wave function at each pixel.

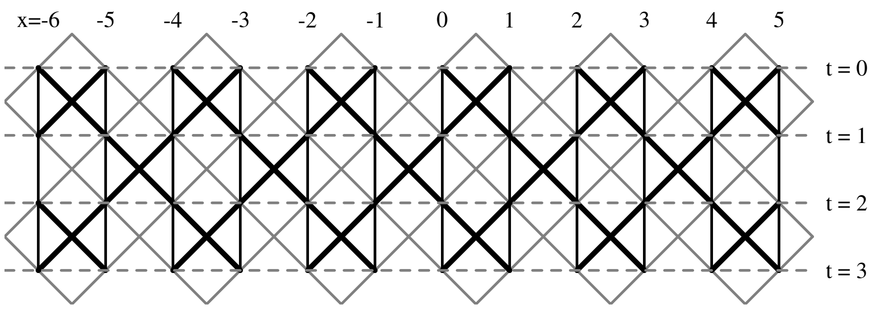

Figure 3: Different sites are paired on alternate time steps.

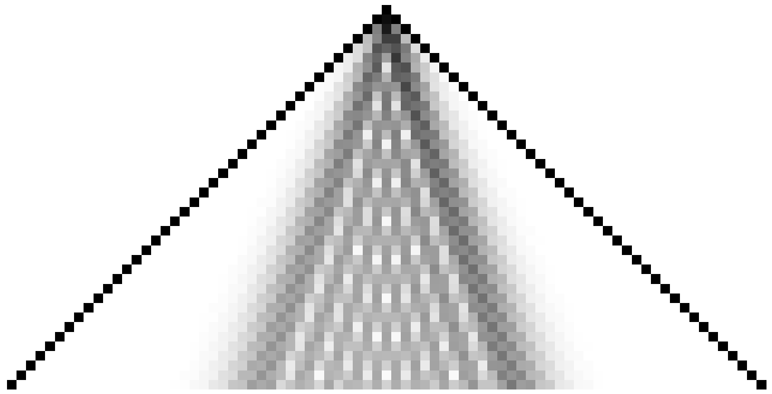

Figure 4: Evolution of δ_0 for $\mu = \pi/8$ with xdim = 84, timesteps = 40. Light cone superinposed in black.

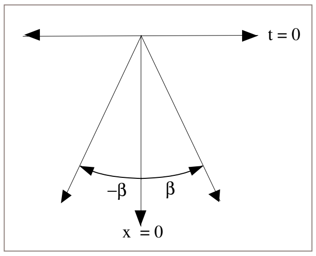

Figure 5: Critical angle β is measured from the vertical axis $x = 0$.

Images such as Figure 4 suggest that there is a critical angle β depending on μ such that:

$$\beta(\mu) = \inf\{\beta \mid \lim_{m,n\to\infty} \{\mathbf{A}^n(\delta_0)\}_m = 0 \text{ whenever } \frac{m}{2n} > \tan(\beta)\} \tag{8}$$

(Note the corrective factor of 2, compensating for the fact that one iteration of $\mathbf{A}$ represents two time steps in the original coordinate system). See Figure 5.

Our main result, which we will demonstrate in the sequel, is:

Theorem 1

$$\tan(\beta(\mu)) \leq \sin(\mu) \tag{9}$$

Strong evidence will be provided that equality holds.

2 On Unitary Operators on $L^2(\mathbf{Z})$ that Commute with T_2

Recall the definition of Fourier transform of a sequence:

$$\hat{s}(\omega) = \sum_{k=-\infty}^{+\infty} s_k e^{-i\omega k} \tag{10}$$

$$s_k = \frac{1}{2\pi}\int_0^{2\pi} \hat{s}(\omega) e^{i\omega k} d\omega \tag{11}$$

As is well known, any bounded operator $\mathbf{A}$ that commutes with T_1 is a convolution operator, that is,

$$\mathbf{A}(s) = F * s, \text{where } F = \mathbf{A}(\delta_0), \tag{12}$$

or equivalently in Fourier space, it is given by a multiplier:

$$\widehat{\mathbf{A}(s)}(\omega) = \hat{F}(\omega) \cdot \hat{s}(\omega) \tag{13}$$

In case $\mathbf{A}$ is unitary, the Fourier multiplier is a phase. As we shall see now, in case $\mathbf{A}$ commutes with T_2 instead of T_1, this phase is replaced by an element of $SU(2, C)$. We now come to the details.

It is obvious that any linear operator that commutes with T_2 is completely determined by its action on the two sequences δ_0 and δ_1 We introduce projections onto the even and odd terms:

$$\{\Pi_e(s)\}_i = \begin{cases} s_i & \text{if i is even} \\ 0 & \text{otherwise} \end{cases}$$

and similarly for the odd projection Π_o. Then $\mathbf{A}$ can be expressed as:

$$\mathbf{A}(s) = \mathbf{A}(\delta_0) * \Pi_e(s) + (T_{-1}\mathbf{A}(\delta_1)) * \Pi_o(s) \tag{14}$$

Let $F_i(\omega) = \widehat{\mathbf{A}(\delta_i)}(\omega)$. Taking the discrete Fourier transform of equation 14 yields:

$$\widehat{\mathbf{A}(s)}(\omega) = F_0(\omega)\widehat{\Pi_e(s)}(\omega) + e^{i\omega}F_1(\omega)\widehat{\Pi_o(s)}(\omega) \tag{15}$$

The next step of our analysis is based on the observation that

$$\{\Pi_e(s)\}_k = \frac{1}{2}((-1)^k s_k + s_k) \tag{16}$$

Replacing -1 by $e^{-i\pi}$ and performing a discrete Fourier transform gives:

$$\begin{aligned} \widehat{\Pi_e(s)}(\omega) &= \frac{1}{2}\sum_{k=-\infty}^{k=\infty}(e^{-ik(\omega+\pi)}s_k + e^{-ik\omega}s_k) \\ &= \frac{1}{2}(\hat{s}(\omega+\pi) + \hat{s}(\omega)) \end{aligned} \tag{17}$$

Doing the same analysis for Π_o yields:

$$\widehat{\Pi_o(s)}(\omega) = \frac{1}{2}(-\hat{s}(\omega+\pi) + \hat{s}(\omega)) \tag{18}$$

Substituting (17) and (18) back into (15) gives finally:

$$\widehat{\mathbf{A}(s)}(\omega) = \frac{1}{2}((\hat{s}(\omega) + \hat{s}(\omega+\pi))F_0(\omega) + (\hat{s}(\omega) - \hat{s}(\omega+\pi))e^{i\omega}F_1(\omega)) \tag{19}$$

We can also compute:

$$\widehat{\mathbf{A}(s)}(\omega+\pi) = \frac{1}{2}((\hat{s}(\omega) + \hat{s}(\omega+\pi))F_0(\omega+\pi) + (\hat{s}(\omega) - \hat{s}(\omega+\pi))e^{i\omega}F_1(\omega+\pi)) \tag{20}$$

Combining (19) and (20), we can express the action of $\mathbf{A}$ on Fourier space as a linear operator $\widehat{\mathbf{A}}$:

$$\begin{pmatrix} \hat{s}(\omega) \\ \hat{s}(\omega+\pi) \end{pmatrix} \mapsto \widehat{\mathbf{A}} \begin{pmatrix} \hat{s}(\omega) \\ \hat{s}(\omega+\pi) \end{pmatrix} \tag{21}$$

where $\widehat{\mathbf{A}}$ is given by the matrix:

$$\frac{1}{2}\begin{pmatrix} F_0(\omega)+e^{i\omega}F_1(\omega) & F_0(\omega)-e^{i\omega}F_1(\omega) \\ F_0(\omega+\pi)+e^{i\omega}F_1(\omega+\pi) & F_0(\omega+\pi)-e^{i\omega}F_1(\omega+\pi) \end{pmatrix} \tag{22}$$

In the sequel, we will let $\widehat{\mathbf{A}} = \widehat{\mathbf{A}}(\omega)$ stand for this matrix. We also introduce the projection operator $\mathbf{P}$ defined by $\mathbf{P}(a,b) = a$, projection onto the first component. Then the iterated dynamic may be obtained through:

$$\widehat{\mathbf{A}^n(s)}(\omega) = \mathbf{P}\left[\widehat{\mathbf{A}}(\omega)^n \begin{pmatrix} \hat{s}(\omega) \\ \hat{s}(\omega+\pi) \end{pmatrix}\right] \tag{23}$$

2.1 Computing Iterates by Inverse Fourier Transform

By Parseval's Theorem, whenever $\mathbf{A}$ is unitary, then so is $\widehat{\mathbf{A}}(\omega)$, that is, $\widehat{\mathbf{A}}(\omega) \in$ U(2,C). Hence, we can change coordinates so that $\widehat{\mathbf{A}}(\omega)$ is diagonal:

$$\widehat{\mathbf{A}}(\omega) = \mathbf{E}(\omega)\mathbf{D}(\omega)\mathbf{E}^{-1}(\omega) \tag{24}$$

where

$$\mathbf{D}(\omega) = k(\omega)\begin{pmatrix} e^{i\lambda(\omega)} & 0 \\ 0 & e^{-i\lambda(\omega)} \end{pmatrix} \tag{25}$$

where $k(\omega)$ is the determinant of $\widehat{\mathbf{A}}$. If, further, $\widehat{\mathbf{A}}$ is special unitary, then $k=1$. In the sequel, we assume this is the case. According to the Fourier inversion theorem, we can reconstruct the m^{th} element of the sequence $\mathbf{A}(s)$ by integrating:

$$\begin{aligned} \{\mathbf{A}(s)\}_m &= \frac{1}{2\pi}\int_0^{2\pi} \mathbf{P}\left[\widehat{\mathbf{A}(s)}(\omega)e^{i\omega m}\begin{pmatrix} \hat{s}(\omega) \\ \hat{s}(\omega+\pi) \end{pmatrix}\right] d\omega \\ &= \frac{1}{2\pi}\int_0^{2\pi} \mathbf{P}\left[\mathbf{E}(\omega)\mathbf{D}(\omega)\mathbf{E}^{-1}(\omega)e^{i\omega m}\begin{pmatrix} \hat{s}(\omega) \\ \hat{s}(\omega+\pi) \end{pmatrix}\right] d\omega \end{aligned} \tag{26}$$

We can just as easily reconstruct the elements of $\mathbf{A}^n(s)$. Equation 26 then becomes:

$$\{\mathbf{A}^n(s)\}_m = \frac{1}{2\pi}\int_0^{2\pi} \mathbf{P}\left[\mathbf{E}(\omega)\mathbf{D}^n(\omega)\mathbf{E}^{-1}(\omega)e^{i\omega m}\begin{pmatrix} \hat{s}(\omega) \\ \hat{s}(\omega+\pi) \end{pmatrix}\right] d\omega \tag{27}$$

We can go further and write this as:

$$\{\mathbf{A}^n(s)\}_m = \frac{1}{2\pi}\int_0^{2\pi} (G_0(\omega)e^{i(n\lambda(\omega)+m\omega)} + G_1(\omega)e^{i(-n\lambda(\omega)+m\omega)})d\omega \tag{28}$$

The functions G_0 and G_1 depend upon μ, F_0, and F_1, but not upon n, and can be computed once, for all n. Writing $\gamma = \frac{m}{n}$, we have

$$\{\mathbf{A}^n(s)\}_m = \frac{1}{2\pi}\int_0^{2\pi} (G_0(\omega)e^{in(\lambda(\omega)+\gamma\omega)}d\omega + \frac{1}{2\pi}\int_0^{2\pi} G_1(\omega)e^{in(-\lambda(\omega)+\gamma\omega)})d\omega \tag{29}$$

For the moment, we focus on the second integral of (29). Define $\phi_\lambda(\omega) = \gamma\omega - \lambda(\omega)$. Then the integrand takes the form $G_1(\omega)e^{in\phi_\lambda(\omega)}$. The theory of asymptotic integrals applies to such integrals and asserts that the integral decays rapidly with n whenever there are no stationary points for the phase, that is, $\phi^{'}(\omega) \neq 0$.

Theorem 2 (Asymptotic Integral [Fed91]) *Let $\{f, \phi\}$ be C^∞ and 2π-periodic. Suppose further that $\phi^{'}(\omega) \neq 0$. Then*

$$\int_0^{2\pi} f(x)e^{i\zeta\phi(x)}dx = O(\zeta^{-m}) \quad (\zeta \to \infty) \tag{30}$$

for all $m > 0$.

Thus, a complete analysis of the asymptotic behavior of the iterates of our original operator $\mathbf{A}$ depends upon computing the critical points of the function $\phi_\gamma(\omega) = \gamma\omega - \lambda(\omega)$, that is, the solutions of

$$\lambda^{'}(\omega) = \gamma \tag{31}$$

2.2 Analysis

We now apply the general formalism to the discrete Dirac operator. We begin our analysis with $\mathbf{A}_e$. We compute:

$$\begin{aligned} F_0(w) &= \cos(\mu) + e^{(-i\omega)} i\sin(\mu) \\ F_1(w) &= i\sin(\mu) + e^{(-i\omega)}\cos(\mu) \end{aligned} \tag{32}$$

We see that the action of $\mathbf{A}_e$ is given in Fourier space in the sense of (22) by the following matrix:

$$\widehat{\mathbf{A}_e} = \begin{pmatrix} \cos(\mu) + i\cos(\omega)\sin(\mu) & \sin(\omega)\sin(\mu) \\ -\sin(\omega)\sin(\mu) & \cos(\mu) - i\cos(\omega)\sin(\mu) \end{pmatrix} \tag{33}$$

Using this and the fact that the shift operator T_1 has a matrix given by:

$$\widehat{T_1} = \begin{pmatrix} e^{-i\omega} & 0 \\ 0 & -e^{-i\omega} \end{pmatrix} \tag{34}$$

we can compute $\widehat{\mathbf{A}} = \widehat{\mathbf{T}_1}\widehat{\mathbf{A}_e}\widehat{\mathbf{T}^*{}_1}\widehat{\mathbf{A}_e}$ explicitly. Rather than give the full form of this, we use the decomposition (24) to write $\widehat{\mathbf{A}} = \mathbf{E}\mathbf{D}\mathbf{E}^{-1}$. In fact, the entries of $\mathbf{D}$ are just the eigenvalues of $\widehat{\mathbf{A}}$ and the columns of $\mathbf{E}$ are just the eigenvectors of $\widehat{\mathbf{A}}$. The eigenvalues of $\widehat{\mathbf{A}}$ are

$$\cos^2(\mu) - \cos(2\ \omega)\sin^2(\mu) \pm 2i\ \cos(\omega)\sin(\mu)\sqrt{\cos(\mu)^2 + \sin(\mu)^2\sin(\omega)^2} \tag{35}$$

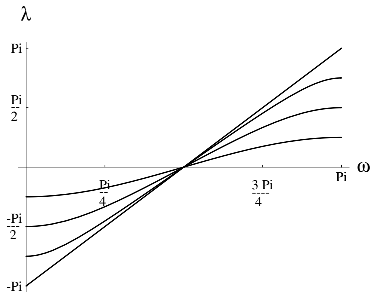

Figure 6: $\lambda(\omega)$ for $\mu \in \{n\pi/8 \mid n = 1, 2, 3, 4\}$

By (25),

$$\mathbf{D}(\omega) = \begin{pmatrix} e^{i\lambda(\mu,\omega)} & 0 \\ 0 & e^{-i\lambda(\mu,\omega)} \end{pmatrix} \tag{36}$$

Equating the real parts of the upper left entries of these two forms, we find:

$$\lambda(\mu, \omega) = -\mathrm{sgn}(\cos(\omega))\ \arccos(\cos^2(\mu) - \cos(2\,\omega)\sin^2(\mu)) \tag{37}$$

In the following we assume the dependence on μ and write simply $\lambda(\omega)$. According to (31) the analysis of the asymptotic behavior of $\mathbf{A}(\delta_0)$ along a line with slope $\gamma = \frac{m}{n}$ with respect to the vertical axis, depends upon the solutions of $\lambda^{'}(\omega) = \gamma$. In particular, if there are no solutions, then the integral (29) decays rapidly.

Figure 6 shows $\lambda(\omega), \omega \in [0, \pi]$ for various values of μ. Note that for $\mu \in (0, \pi/2)$, the graphs all have local minimums at $\omega = 0$ and a single local maximum at $\omega = \pi$, where $\omega^{'} = 0$. Furthermore, these graphs are all odd with respect to a zero at $\omega = \pi/2$, that is, $\lambda(\omega) = -\lambda(\pi - \omega)$. In fact there is a single inflection point at $\lambda = \pi/2$, where the derivative $\lambda^{'}$ attains its maximal value. Hence the graph of $\lambda^{'}$ is convex and symmetric with respect to $\omega = \pi/2$, so any horizontal line cuts it in exactly two points or not at all. Theorem 2 then implies that whenever $\gamma > \lambda^{'}(\pi/2)$, the integral (29) decays rapidly, which explains the finite propagation speed measured by the apparent opening angle β. If $\gamma \leq \lambda^{'}(\pi/2)$, there is no *a priori* reason for the integral to decay fast. More work remains to establish the behavior of the two solutions of (31) with respect to this integral. The computer evidence strongly suggests that the inequality in Theorem 1 is sharp.

In order to compute the asymptotic angle, we differentiate (37):

$$\lambda^{'}(\omega) = \frac{-2\sin^2(\mu)\sin(2\omega)}{\sqrt{1 - (\cos^2(\mu) - \cos(2\omega)\sin^2(\mu))^2}} \tag{38}$$

We are interested in $\lambda^{'}(\pi/2)$ since this will yield the extreme value ω_c of ω for which the integral (29) does not vanish. Although both top and bottom vanish at $\omega = \pi/2$, it is possible to evaluate using L'Hopital's rule, and the result is $\lambda^{'}(\pi/2) = 2\sin(\mu)$. As noted previously, the factor of 2 appears because we are analysing the operator $\mathbf{A}$, which represents 2 time steps of the original system. When we reparametrize Figure 5 to take this into account, Theorem 2 is proved.

3 Conclusions

We have described a discrete version of the one-dimesional Dirac equation and shown how to compute the asymptotic behavior of the system. This analysis is based on results generally valid for unitary operators on $L^2(\mathbf{Z})$ which commute with translation by two: The Fourier version of such operators can be represented by elements of $SU(2, C)$, and the Fourier inversion integral combined with a weak form of the Asymptotic Integral Theorem allows us to compute the critical angle for the Dirac system under consideration.

More work remains to be done to evaluating the integral (29) for values of $\omega < \omega_c$. Such work should lead to an understanding of the interference patterns seen in Figure 4, as well as establishing equality in Theorem 1. Higher-order techniques are required to carry out an analysis of the scaling behavior of the wave-front $(\omega = \omega_c)$. Also, the discrete version of the two dimensional Dirac equation should be accessible to a similar analysis.

References

[Fed91] Fedoryukivich Fedoryuk. *Asymptotic Analysis.* Academic Press, 1991.