Counting $S(\Delta k, \Delta w)$ at $\beta = 0$ in the XX Model

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October 2019

1 Setup

1.1 The lattice

Consider a discrete lattice with lattice spacing $a = 1$ and an even integer $L > 0$ lattice points.

In Fourier space, the only allowed k values are $k = \frac{2\pi d}{L}$ for $d \in \mathbb{Z}$. Note that because L is even, $k = 0$ and $k = \pi$ will both be included. We can also consider k_1, k_2 equivalent if $k_1 - k_2 = 2\pi d$ for some integer d.

The dispersion relation goes as $w = cos(k)$.

1.2 Defining $S(\Delta k, \Delta w)$

I will calculate $S(\Delta k, \Delta w)$ at infinite temperature ($\beta = 0$). This is represented below:

$$S(\Delta k, \Delta w) = \sum_{uv} \delta(\Delta w - (E_u - E_v)) \| \langle u | S^z_{\Delta k} | v \rangle \|^2 \tag{1}$$

Here, $|u\rangle, |v\rangle$ represent states in the sum of Hilbert spaces from 0 to L particles. At infinite temperature, all 2^L states are equally likely.

The $\| \langle u | S^z_{\Delta k} | v \rangle \|^2$ term describes a transition from state $|u\rangle$ to state $|v\rangle$, with change in total momentum Δk. This term should conserve total particle number.

1.3 Allowed values of Δk and Δw

We define S^z_k below:

$$S^z_{\Delta k} = \sum_k a^\dagger_k a_{k+\Delta k} \tag{2}$$

This operator can be described by annihilating a particle at momentum $k + \Delta k$ and creating a particle at momentum k. State transitions can only change particle momentum by Δk.

So we only need to consider transitions of a single particle moving in (k, w)-space, from $(m, cos(\frac{2m\pi}{L}))$ to $(n, cos(\frac{2n\pi}{L}))$. This restricts Δk:

$$\Delta k = \frac{2\pi d}{L}, d \in \mathbb{Z} \tag{3}$$

There are some interesting symmetries. Since k_1 is equivalent to $k_2 = k_1 + 2\pi d$ for integer d, Δk and $\Delta k'$ can be thought of as equivalent when $k - k' = 2\pi d$ for integer d. This corresponds to one-particle transitions from the same initial k_1 to k_2 in different Brillouin zones.

Additionally, there is a reflection symmetry around the w-axis. We could consider transitions to the "right" or to the "left" without loss of generality. So, Δk and $-\Delta k$ can be thought of as equivalent.

Thus, we only need to compute Δk from 0 to π.

The $\delta(\Delta w - (E_m - E_n))$ term restricts $S(\Delta k, \Delta w)$ nonzero only at Δw corresponding to transitions:

$$\Delta w = cos(\frac{2m\pi}{L}) - cos(\frac{2n\pi}{L}), n, m \in \mathbb{Z} \tag{4}$$

2 Doing the counting

2.1 Each one-particle transition can be done 2^{L-2} equally likely ways

Suppose you transition a particle from k_1 to k_2. Before you make the transition, you need the input k_1 filled and the output k_2 empty. You have 2^{L-2} total choices when specifying the other k-values.

Each transition uniquely specifies a state; it takes the starting state, empties the input k_1 and fills the output k_2. So, there are $2^{L-2} \cdot 1 = 2^{L-2}$ ways to jump from k_1 to k_2.

Each jump is equally likely because all states are equally likely at infinite temperature.

2.2 Choosing $\Delta k \neq 0, \Delta w$ specifies 0, 1, or 2 distinct one-particle transitions

If Δk or Δw are not allowed, there are 0 one-particle transitions.

Suppose the Δk and Δw are allowed by a transition from (k_1, w_1) to (k_2, w_2) where $k_1 \neq k_2$. By symmetry of $cos(k)$, there exist points $(\pi - k_1, -w_1)$ and $(\pi - k_2, -w_2)$. A transition from $\pi - k_2$ to $\pi - k_1$ would have the same $\Delta k = \pi - k_1 - (\pi - k_2) = k_2 - k_1$ and $\Delta w = -w_1 - (-w_2) = w_2 - w_1$. This second transition is distinct except when both $\Delta w = 0$ and $k_1 + k_2 = \pi \mod 2\pi$.

In other words, any (Δk, Δw) has 2 distinct one-particle transitions, except for nonzero Δw where the transition is symmetric about the k-axis. (*Note: As we will see, for every Δk, the number of exception Δw goes as $1/L$.*)

I have not formally proved uniqueness, i.e. there are at most 2 distinct one-particle transitions. Perhaps it can be done by thinking about the average of $sin(x)$ over a sliding window somewhere in the domain 0 to $\frac{\pi}{2}$.

2.3 Computing allowed values of $\Delta w(\Delta k)$

We can simplify equation 4 using the trigonometric sum-difference formulas:

$$\Delta w = cos(\frac{2m\pi}{L}) - cos(\frac{2n\pi}{L}) = 2sin(\frac{2\pi}{L}\frac{(m+n)}{2})sin(\frac{2\pi}{L}\frac{(m-n)}{2}), n, m \in \mathbb{Z} \tag{5}$$

Since the associated $\Delta k = \frac{2\pi(m-n)}{L}$, we can find the allowed $\Delta w(\Delta k)$:

$$\Delta w(\Delta k) = 2sin(\frac{2\pi m}{L} - \frac{\Delta k}{2})sin(\frac{\Delta k}{2}) = sin(\frac{2\pi m}{L})sin(\Delta k) - cos(\frac{2\pi m}{L})(1 - cos(\Delta k)), m \in \mathbb{Z} \tag{6}$$

In general, since $e^{icx} = cos(cx) + isin(cx)$, $Acos(cx) + Bsin(cx)$ represents a sinusoid:

$$Acos(cx) + Bsin(cx) = Re((A - iB)e^{icx}) = \sqrt{A^2 + B^2} cos(cx - \arctan \frac{B}{A}) \tag{7}$$

We can verify that the allowed $\Delta w(\Delta k)$ are points from a sinusoid with a phase shift:

$$\Delta w(\Delta k) = \sqrt{(cos(\Delta k) - 1)^2 + sin^2(\Delta k)} cos(\frac{2\pi m}{L} - \arctan \frac{sin(\Delta k)}{cos(\Delta k) - 1}), m \in \mathbb{Z} \tag{8}$$

$$\Delta w(\Delta k) = \sqrt{2 - 2cos(\Delta k)} cos(\frac{2\pi m}{L} - \frac{\pi + \Delta k}{2}) = 2sin(\frac{\Delta k}{2}) sin(\frac{2\pi m}{L} - \frac{\Delta k}{2}), m \in \mathbb{Z} \tag{9}$$

2.4 Degeneracy of $\Delta w(\Delta k)$

This function takes up to L distinct values: Each starting point (position m) on the lattice could produce a different Δw.

When $\Delta k = 0$, only $\Delta w = 0$ is allowed, so it has degeneracy L.

For nonzero Δk, there are at most two starting positions $m \neq 0$ that change from k_m to $-k_m$. Those two points will have degeneracy 1, and the rest will have degeneracy 2.

In particular, there exists a starting position m with $w_m = 0$ if and only if L is divisible by 4. In these cases, only Δk corresponding to an odd number of steps $s = 2d + 1, d \in \mathbb{Z}$ will have two points with degeneracy 1 (d steps above and below the zero position).

The opposite is true for L even but not divisible by 4: Only Δk corresponding to an even (nonzero) number of steps $s = 2d, d \in \mathbb{Z}$ will have two points with degeneracy 1 (d steps above and below $w = 0$).

All together:

$$count(\Delta w = 0, \Delta k = 0, L) = L \tag{10}$$

And considering $d, e \in \mathbb{Z}$:

$$count(\Delta w = \pm 2sin(\frac{2\pi d}{L}), \Delta k = \frac{2(2d + 1)\pi}{L}, L = 4e) = 1 \tag{11}$$

$$count(\Delta w = \pm 2sin(\frac{2\pi d - \pi}{L}), \Delta k = \frac{4d\pi}{L} \neq 0, L = 4e + 2) = 1 \tag{12}$$

And in all other allowed cases, $count(\Delta w, \Delta k, L) = 2$.

2.5 Calculating $S(\Delta k, \Delta w)$

Using the previous section:

$$S(\Delta k, \Delta w) = \delta_{e^{ikL}-1} \delta_{\Delta w - \Delta w(\Delta k)} count(\Delta w, \Delta k, L) \frac{2^{L-2}}{2^L} = \frac{1}{4} \delta_{e^{ikL}-1} \delta_{\Delta w - \Delta w(\Delta k)} count(\Delta w, \Delta k, L) \tag{13}$$

In this form, it is hard to visualize, but let me sketch a few details.

- Δk is fixed on a grid. and S is symmetric about Δk and periodic with $\Delta k = 2\pi$.
- Δw is only allowed at certain values for each Δk, described by equation 6.
- The value of S at each allowed (k, w) is uniform except for a few cases, dependent on L and Δk.

3 Features of $\Delta w(\Delta k)$

3.1 Computing the minimum allowed $|\Delta w(\Delta k)|$

If Δk corresponds to an even number of steps in k, the jump can be symmetric around $k = 0$ (so $\Delta w = 0$).

If Δk corresponds to an odd number of steps $s = 2d + 1$ in k, the jump must be nonzero. It is best to have the endpoints nearest to $k = 0$ (where the slope of $w(k)$ is the smallest). For $0 \leq s \leq L/2$ (the relevant range) this implies centering around $k = 0$. So, the minimum jump will be $cos(2d\pi/L) - cos(2(d+1)\pi/L)$.

All together:

$$min|\Delta w(\Delta k)| = 0, \Delta k = \frac{4d\pi}{L}, d \in \mathbb{Z} \tag{14}$$

$$min|\Delta w(\Delta k)| = cos(\frac{2d\pi}{L}) - cos(\frac{2(d+1)\pi}{L}), \Delta k = \frac{2(2d+1)\pi}{L}, d \in \mathbb{Z} \tag{15}$$

The above formula could be rewritten in trigonometric functions of $\frac{2\pi}{L}$ and $\frac{2d\pi}{L}$, if the reader is interested.

3.2 Computing the maximum allowed $\Delta w(\Delta k)$

When $\Delta k = 0$, $\Delta w = 0$. The rest of the subsection explores $\Delta k \neq 0$.

Suppose L is divisible by 4. Then there will be a point at $w = 0$. The maximum Δw corresponds to the largest jump around $w = 0$ (where the slope of $w(k)$ is largest in magnitude). So, for an odd number of lattice steps $s = 2d+1, d \in \mathbb{Z}$, the maximum is $sin(\frac{2\pi d}{L}) - sin(-\frac{2\pi d}{L}) = 2sin(\frac{2\pi d}{L}))$. For an even number of lattice steps $s = 2d, d \in \mathbb{Z}$ it's nearly that: $sin(\frac{2\pi(d-1)}{L}) - sin(-\frac{2\pi d}{L}) = sin(\frac{2\pi d}{L}) + sin(\frac{2\pi(d-1)}{L})$.

When L is even but not divisible by 4, there is no point at $w = 0$. The best case is when Δk corresponds to an even number of lattice steps $s = 2d, d \in \mathbb{Z}$; then, the maximum is $sin(\frac{2\pi d - \pi}{L}) - sin(\frac{-2\pi d + \pi}{L}) = 2sin(\frac{2\pi d - \pi}{L})$. When Δk is an odd number of lattice steps $s = 2d+1, d \in \mathbb{Z}$, the maximum is $sin(\frac{2\pi d - \pi}{L}) - sin(-\frac{2\pi d - \pi}{L}) = sin(\frac{2\pi d - \pi}{L}) + sin(\frac{2\pi d + \pi}{L}) = 2sin(\frac{2\pi d}{L})cos(\frac{\pi}{L})$.

All together, assuming $d, e \in \mathbb{Z}$:

$$max\Delta w(\Delta k) = 2sin(\frac{2\pi d}{L}), \Delta k = \frac{2\pi(2d+1)}{L}, L = 4e \tag{16}$$

$$max\Delta w(\Delta k) = sin(\frac{2\pi d}{L}) + sin(\frac{2\pi(d-1)}{L}), \Delta k = \frac{4\pi d}{L} \neq 0, L = 4e \tag{17}$$

$$max\Delta w(\Delta k) = 2sin(\frac{2\pi d}{L})cos(\frac{\pi}{L}), \Delta k = \frac{2\pi(2d+1)}{L}, L = 4e+2 \tag{18}$$

$$max\Delta w(\Delta k) = 2sin(\frac{2\pi d - \pi}{L}), \Delta k = \frac{4\pi d}{L} \neq 0, L = 4e+2 \tag{19}$$

3.3 Computing the average allowed $|\Delta w(\Delta k)|$ as $L \to \infty$

In the thermodynamic limit, the average allowed $|\Delta w(\Delta k)|$ can be found by averaging its expression:

$$|\Delta w(\Delta k)| = |2sin(\frac{\Delta k}{2})sin(\frac{2\pi m}{L} - \frac{\Delta k}{2})| = \frac{4}{\pi}sin(\frac{\Delta k}{2}) \tag{20}$$

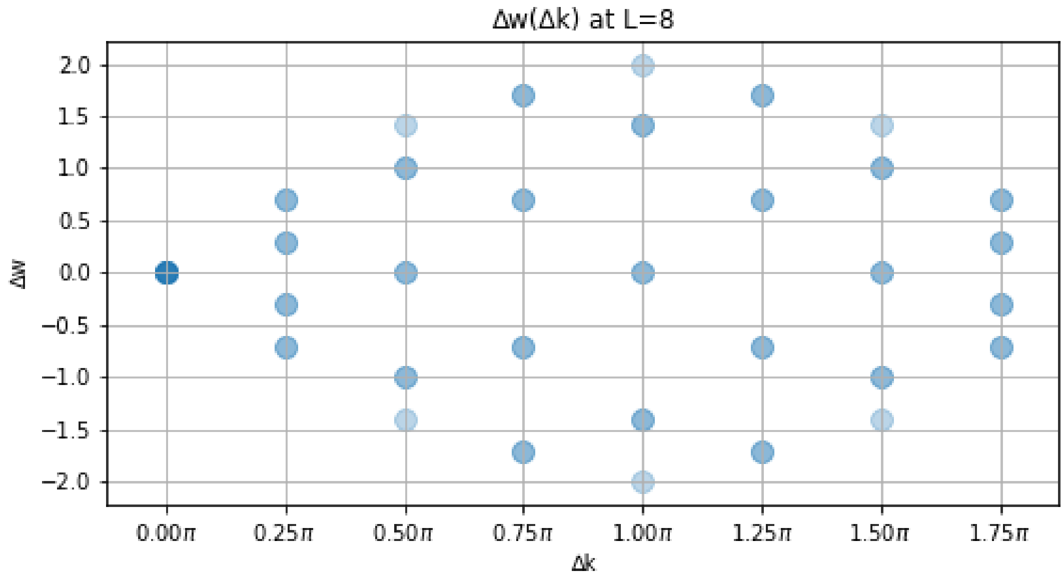


Figure 1: $\Delta w(\Delta k)$ at $L = 8$. The plot is symmetric about $\Delta k = \pi$ and $\Delta w = 0$.

4 Plots

4.1 Plotting $\Delta w(\Delta k)$ at various L

We know a few details about this function so far:

- The minimum of $|\Delta w|$ stays around zero.
- The maximum of Δw goes roughly as $2sin(\frac{\Delta k}{2})$.
- The average $|\Delta w|$ goes roughly as $\frac{4}{\pi}sin(\frac{\Delta k}{2})$.

Figures 1, 2, 3, 4 visualize $\Delta w(\Delta k)$ at various L. The generating code is in a Jupyter notebook and PDF attached to this project.

Ignoring nearly uniform degeneracies, $\Delta w(\Delta k)$ can be used to describe the density of states of $S(\Delta k, \Delta w)$, especially as $L \to \infty$. I use alpha compositing on these plots to better show this density of states.

4.2 Plotting $S(\Delta k, \Delta w)$ at various L and Δk

At finite L, this function is a summation of Kronecker delta functions at allowed $(\Delta k, \Delta w)$ values. So, for these plots, I convert allowed values of $(\Delta k, \Delta w)$ to Gaussians with $\sigma_{\Delta w} = 0.1$.

Figures 5a, 5b visualize S at various Δk. The density of states is similar to the output $y = sin(x)$ sampled at fixed x, so S is similar to the curve $\frac{d}{dx} \arcsin x = \frac{1}{\sqrt{1-x^2}}$.

Figures 6a, 6b, 6c visualize S at various L. The oscillations disappear at larger L, but that threshold increases with increasing Δk.

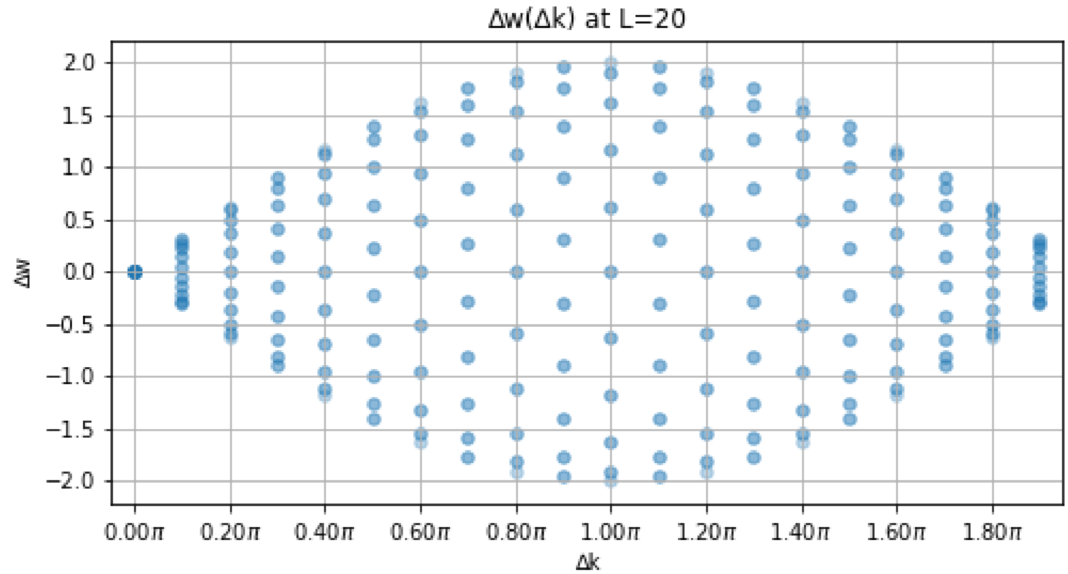


Figure 2: $\Delta w(\Delta k)$ at $L = 20$. Notice how the maximum goes approximately with $2sin(\frac{\Delta k}{2})$.

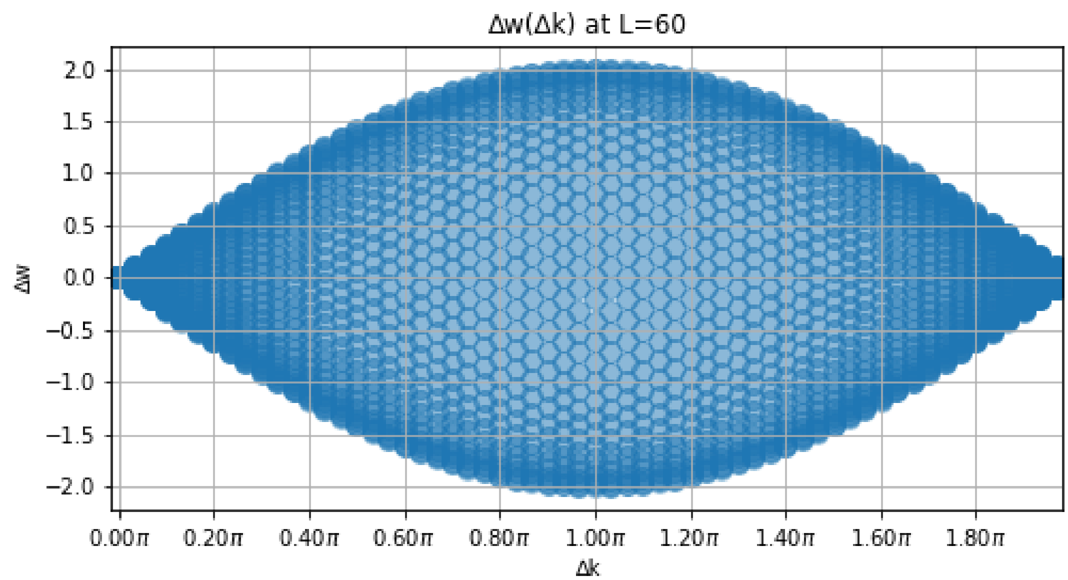


Figure 3: $\Delta w(\Delta k)$ at $L = 60$. The darker areas correspond to a higher density of states (thus a higher $S(\Delta k, \Delta w)$). Although Δw can vary across the plot, many states are concentrated around the maximum $|\Delta w(\Delta k)|$.

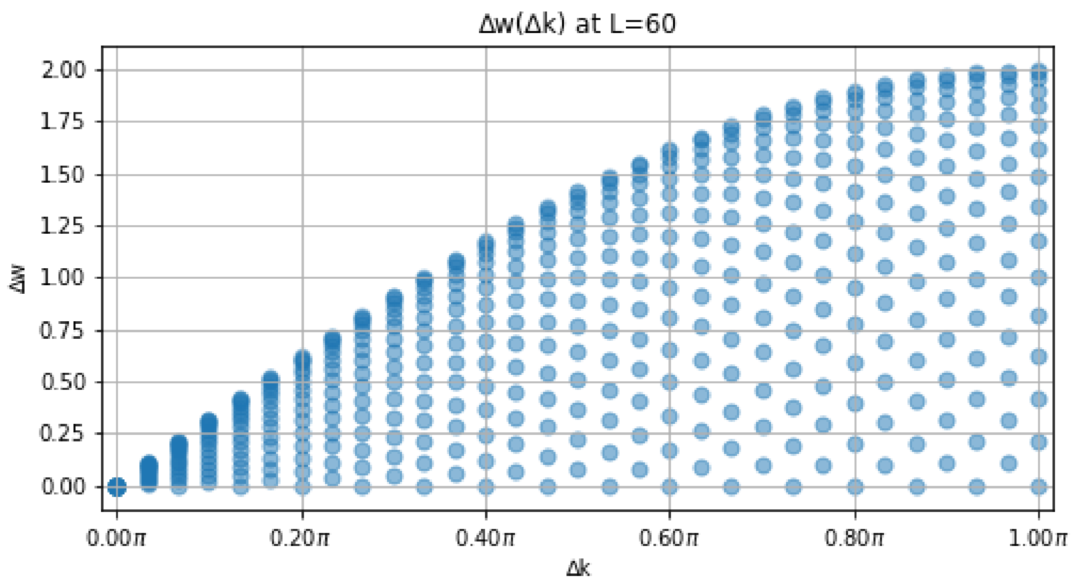
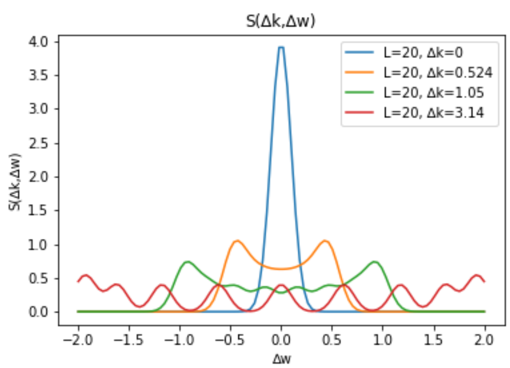
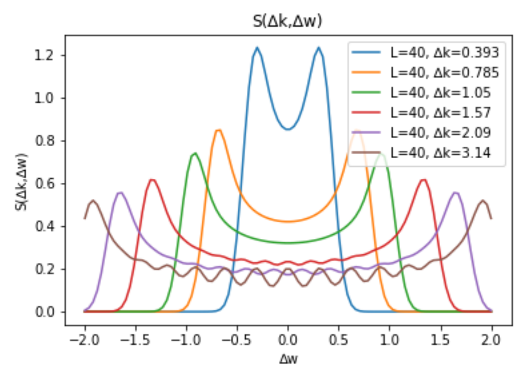


Figure 4: Quarter-plot of $\Delta w(\Delta k)$ at $L = 60$. This function is symmetric about both the Δk-axis and Δw-axis. Notice that every other allowed Δk includes $\Delta w = 0$.

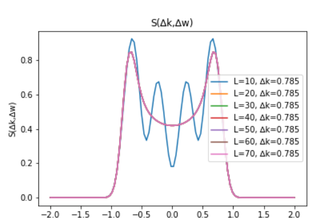


(a) $S(\Delta k, \Delta w)$ at $L = 20$.

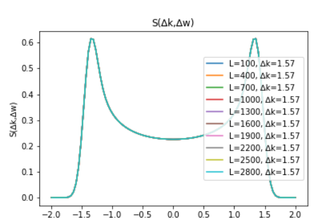


(b) $S(\Delta k, \Delta w)$ at $L = 40$.

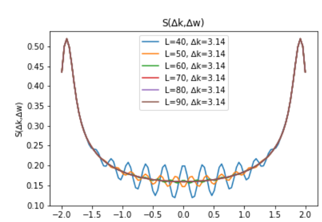
Figure 5: Plot of $S(\Delta k, \Delta w)$ at various Δk. At higher Δk, the function requires higher L to smooth out.



(a) $S(\Delta k, \Delta w)$ at $\Delta k = 0.25\pi$.



(b) $S(\Delta k, \Delta w)$ at $\Delta k = 0.5\pi$.



(c) $S(\Delta k, \Delta w)$ at $\Delta k = \pi$.

Figure 6: Plot of $S(\Delta k, \Delta w)$ at various L. The function stabilizes as $L > 50$.

5 Examples

5.1 Worked example: L=2

If there are only 2 elements in the lattice, then only $(k = 0, w = 1)$ and $(k = \pi, w = -1)$ are allowed. So, there are 4 distinct one-particle transitions:

1. $k = 0 \to k = 0$ $(\Delta k = 0, \Delta w = 0)$
2. $k = 0 \to k = \pi$ $(\Delta k = \pi, \Delta w = -2)$
3. $k = \pi \to k = 0$ $(\Delta k = \pi, \Delta w = 2)$
4. $k = \pi \to k = \pi$ $(\Delta k = 0, \Delta w = 0)$

This matches each analytical result:

- There are 0-2 one-particle transitions per $(\Delta k, \Delta w)$
- $\Delta w(0) = 0$
- $\Delta w(\pi) = sin(\frac{2\pi m}{L}) = \pm 1$
- The reader can verify that minimum and maximum allowed $|\Delta w|$ match at both $\Delta k = 0$ and $\Delta k = \pi$.

5.2 Worked example: L=4

With four points on the lattice, there are four points in k-space: $(k, w) \in \{(0, 1), (\frac{\pi}{2}, 0), (\pi, -1), (\frac{3\pi}{2}, 0)\}$. Consider the distinct transitions with positive Δk:

- $\Delta k = 0$. Here, $\Delta w = 0$ for all 4 possibilities.
- $\Delta k = \frac{\pi}{2}$. Here, in two cases $(k = \pi, \frac{3\pi}{2})$, $\Delta w = 1$, and in the other two, $\Delta w = -1$.
- $\Delta k = \pi$. Here, in two cases $(k = \frac{\pi}{2}, \frac{3\pi}{2})$, $\Delta w = 0$, and the other two cases produce $\Delta w = \pm 2$.
- $\Delta k = \frac{3\pi}{2} = \frac{-\pi}{2} + 2\pi$. This has the same behavior as $\Delta k = \frac{\pi}{2}$.

This again matches each analytical result, including:

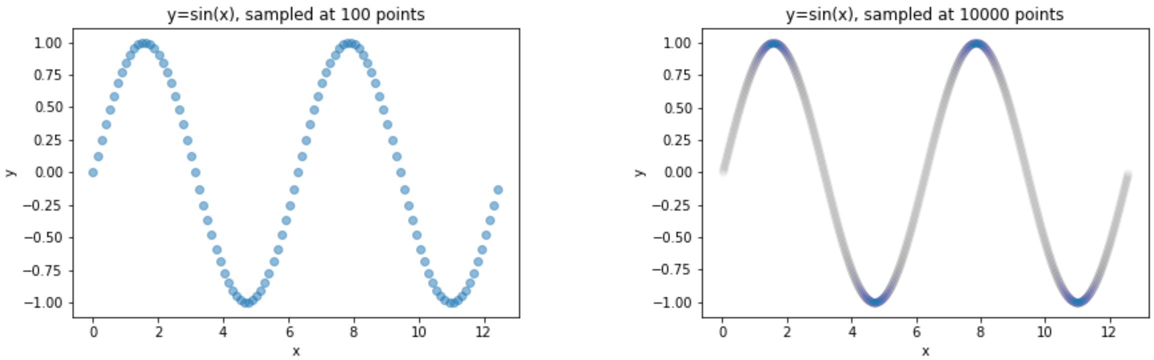
- There are 0-2 one-particle transitions per $(\Delta k, \Delta w)$
- $\Delta w(\frac{\pi}{2}) = cos(\frac{2\pi m}{L}) + sin(\frac{2\pi m}{L}) = \pm 1$
- The reader can verify the degeneracies are in the expected places.

5.3 Worked example: L=8

With eight points on the lattice, there are the same four points in k-space as in $L = 4$, and four new points: $\{(\frac{\pi}{4}, \frac{\sqrt{2}}{2}), (\frac{3\pi}{4}, -\frac{\sqrt{2}}{2}), (\frac{5\pi}{4}, -\frac{\sqrt{2}}{2}), (\frac{7\pi}{4}, \frac{\sqrt{2}}{2})\}$. Considering transitions where $0 \leq \Delta k \leq \pi$:

- $\Delta k = 0$. This forces $\Delta w = 0$ for all L starting positions.
- $\Delta k = \frac{\pi}{4}$. This has $\Delta w = \pm\frac{\sqrt{2}}{2}, \pm(1 - \frac{\sqrt{2}}{2})$.
- $\Delta k = \frac{\pi}{2}$. This has $\Delta w = \pm 1, 0$, and one value each $(k = \frac{\pi}{4}, \frac{5\pi}{4})$ with $\Delta w = \pm\sqrt{2}$.
- $\Delta k = \frac{3\pi}{4}$. This has $\Delta w = \pm\frac{\sqrt{2}}{2}, \pm(1 + \frac{\sqrt{2}}{2})$.
- $\Delta k = \pi$. This has $\Delta w = \pm 2, 0$, and one value each $(k = \frac{\pi}{4}, \frac{5\pi}{4})$ with $\Delta w = \pm\sqrt{2}$.

The reader can compare these values to Figure 1.



(a) $y = sin(x)$, sampled 100 times in 4π.

(b) $y = sin(x)$, sampled 10000 times in 4π.

Figure 7: Plot of $y = sin(x)$, sampled evenly in x. Most points have $|y| \approx 1$.

6 Asymptotic behavior of $S(\Delta k, \Delta w)$ as $L \to \infty$

6.1 Using $\Delta w(\Delta k)$ as a density of states

In equation 6, each transition of a particular Δk gives a Δw depending on the starting position m. In the thermodynamic limit, $L \to \infty$, which increases the number of distinct starting positions m. To get a sense of the value at $S(\Delta k, \Delta w_0)$, it's crucial to know how many starting positions m give Δw in a nearby range.

Consider an example $y = sin(x)$ for some $x \in \mathbb{R}$. Intuitively, sampling y at mx at each $m \in \mathbb{Z}$ will produce more points in the "peaks" and "valleys" of $sin(x)$, since the slope of y is so large near $y = 0$ (in fact, its magnitude is close to $cos(0) = 1$). Figure 7 illustrates this.

More formally, the value of $S(\Delta k, \Delta w_0)$ depends on the proportion of m that produce $\Delta w \in [\Delta w_0, \Delta w_0 + \epsilon)$. In the simple example, $x = \arcsin y$ describes the inputs required to produce some y-value. To find how many x-values are captured by a change in y-value, we use the derivative:

$$\rho(y) = \frac{dx}{dy} = \frac{d}{dy} \arcsin y = \frac{1}{\sqrt{1 - y^2}} \tag{21}$$

Figure 8 compares a histogram of samples of $sin(x)$ with equation 21.

6.2 $S(\Delta k, \Delta w)$ as $L \to \infty$

For each Δk, the value of $S(\Delta k, \Delta w)$ is proportional to $\frac{dm}{d(\Delta w(\Delta k))}$. (Remember that equation 6 takes a value at every $m \in \mathbb{Z}$.) This can be directly computed:

$$\frac{dm}{d\Delta w(\Delta k)} \propto \frac{d}{d\Delta w}\left(\frac{\Delta k}{2} + \arcsin \frac{\Delta w}{2 \sin(\Delta k/2)}\right) = \frac{1}{\sqrt{4 \sin^2(\Delta k/2) - (\Delta w)^2}} \tag{22}$$

At small Δk, this equation simplifies to $\left((\Delta k)^2 - (\Delta w)^2\right)^{-1/2}$. The reader can look to plots in Figures 5, 6 which exhibit this behavior.

7 Acknowledgements

Thanks to Nick Sherman for posing the problem to me and answering my many questions.

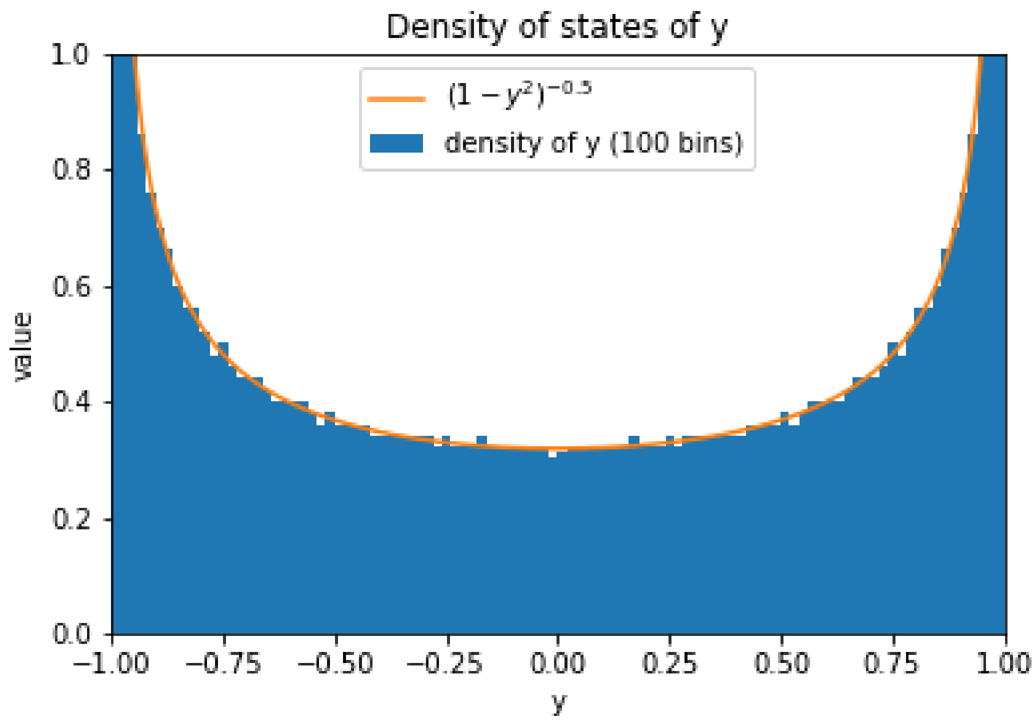


Figure 8: Distribution of y-values of $y = sin(x)$, sampled evenly in x. As the number of samples goes to ∞, the distribution $\rho(y)$ approaches $\frac{d}{dy} \arcsin y$. At each Δk, $\Delta w(\Delta k)$ and $S(\Delta k, \Delta w)$ are similarly related. In the thermodynamic limit, $S(\Delta k, \Delta w)$ approaches a value proportional to $\frac{d}{d(\Delta w)} \arcsin \Delta w = \frac{1}{\sqrt{1-(\Delta w)^2}}$.