Manual Link Target Test

Debugging Test

May 2, 2025

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Physics 415 - Lecture 1: Statistical Mechanics (Preview)

January 22, 2025

In statistical mechanics, we will be interested in the laws governing the behavior of "macroscopic" systems.

- Macroscopic = composed of many constituent particles (atoms, molecules, etc.)
- Typical # $\sim 10^{23}$ particles.

In principle, if "microscopic" (M-scopic) laws are known, then properties of systems of a large # of particles can be deduced by solving the M-scopic equations.

Example: Classical system of N particles:

$$m_i \ddot{\vec{r}}_i = \vec{F}_i(\vec{r}_1, \ldots, \vec{r}_N), \quad i = 1, \ldots, N$$

(where $\dot{} \equiv \frac{d}{dt}$, $\ddot{} \equiv \frac{d^2}{dt^2}$, etc.) Given initial conditions $\vec{r}_i(t=0)$ and $\vec{v}_i(t=0)$ ($\vec{v}_i = \dot{\vec{r}}_i$), we have complete knowledge of the state of the system at any time t.

However, for macroscopic N ($N \sim 10^{23}$), this is not feasible.

- Even if we could solve the equations of motion (EOM), simply recording all initial conditions is not practical.
- Indeed, knowing the state of each particle is not even useful or interesting info.
- When the # of particles is large, we'd rather have info about the "average" properties of the system.

Thus, in statistical mechanics, we will abandon such M-scopic determinism in favor of a statistical (or probabilistic) description.

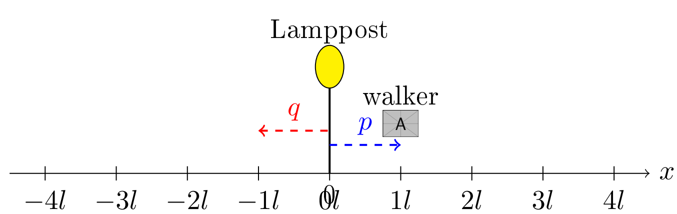
We will find that, precisely because of the large # of particles involved, new laws & types of regularities will appear that govern the macroscopic behavior.

- Notions like "entropy" & "temperature" will emerge, that have no analog in particle mechanics & are purely of statistical nature.

Since statistical notions will be important for understanding macroscopic systems, we'll spend some time reviewing basics of probability. This will be mostly math (not physics). We'll illustrate important ideas through an important example:

1D Random Walk

(A good starting point for understanding a variety of phenomena).



- Walker starts from lamppost at $x = 0$.
- Taking random steps of length l at regular intervals.
- Each step is independent of the last.
- Probability p to step to the right & probability $q = 1 - p$ to step to the left.

Question: After taking N steps, what is the probability that the walker is at a position $x = ml$ (m = integer)? (For another example of a 1D random walk, see "probability board" demo at Ingersoll museum).

We want to calculate the probability $P_N(m)$ that the walker is at position $x = ml$ after N steps.

- Let $n_1 = \#$ of steps right, $n_2 = \#$ of steps left.
- Total steps: $N = n_1 + n_2$.
- Final position: $ml = n_1 l - n_2 l \implies m = n_1 - n_2$.
- Note: $-N \leq m \leq N$. Also, N and m must have the same parity ($N - m = 2n_2$ is even).
- From the above, we can express n_1 and n_2 in terms of N and m: $n_1 = (N + m)/2$ $n_2 = (N - m)/2$

The probability of taking a specific sequence of n_1 steps right and n_2 steps left is:

$$(\underbrace{p \times p \times \cdots \times p}_{n_1 \text{ times}}) \times (\underbrace{q \times q \times \cdots \times q}_{n_2 \text{ times}}) = p^{n_1} q^{n_2}$$

Of course, there are many different ways (sequences) in which the walker could take n_1 steps right & n_2 steps left.

Example: $N = 3$, $m = 1$. Then $n_1 = (3+1)/2 = 2$, $n_2 = (3-1)/2 = 1$. Possible sequences: a) $\rightarrow\rightarrow\leftarrow$ b) $\rightarrow\leftarrow\rightarrow$ c) $\leftarrow\rightarrow\rightarrow$ There are 3 ways.

In general, the number of ways is given by the binomial coefficient:

$$\# \text{ of ways} = \binom{N}{n_1} = \frac{N!}{n_1!(N - n_1)!} = \frac{N!}{n_1! n_2!}$$

Check above example: $N = 3, n_1 = 2, n_2 = 1 \implies \binom{3}{2} = \frac{3!}{2!1!} = 3$. ✓

Therefore, the total probability $P_N(m)$ is (number of ways) $\times$ (probability of one way):

$$P_N(m) = \frac{N!}{n_1! n_2!} p^{n_1} q^{n_2}$$

This is the "binomial distribution".

Using $n_1 = (N + m)/2$ and $n_2 = (N - m)/2$:

$$P_N(m) = \frac{N!}{[(N + m)/2]![(N - m)/2]!} p^{(N+m)/2} (1 - p)^{(N-m)/2}$$

Recall the binomial theorem: $(p + q)^N = \sum_{n_1=0}^{N} \frac{N!}{n_1!(N-n_1)!} p^{n_1} q^{N-n_1}$. Comparing with the formula for $P_N(m)$ (summed over n_1 or m) explains the name.

Example: $p = q = 1/2$ (unbiased walk).

$$P_N(n_1) = \frac{N!}{n_1! n_2!} \left(\frac{1}{2}\right)^N$$

Let's consider $N = 10$. The probability $P_{10}(n_1)$ is plotted below. Note: $m = n_1 - n_2 = n_1 - (N - n_1) = 2n_1 - N$.

n_1	Approx $P_{10}(n_1)$
0	≈ 0.001
1	≈ 0.01
2	≈ 0.044
3	≈ 0.12
4	≈ 0.21
5	≈ 0.25

After $N = 10$ steps, probability is largest for the particle to be near the origin ($m = 0$, or $n_1 = 5$). Probability to be far from the origin is small.

General Notions

Let X be a random variable, taking K possible values $x_1, x_2, \dots, x_K$, with associated probabilities $P(x_1), P(x_2), \dots, P(x_K)$. ($0 \le P(x_i) \le 1$ and $\sum_{i=1}^{K} P(x_i) = 1$).

Mean

The "mean" (average) of X is: $\overline{X} = \sum_{i=1}^{K} P(x_i)x_i$. For a function $f(X)$: $\overline{f(X)} = \sum_{i=1}^{K} P(x_i)f(x_i)$.

Variance

Suppose we want to know how much measurements of X "fluctuate" about the mean value. The "variance" (second moment, dispersion) is defined as:

$$\mathrm{Var}(X) = \sigma_X^2 = \overline{(X - \overline{X})^2} = \sum_{i=1}^{K} P(x_i)(x_i - \overline{X})^2$$

We square the deviation $(x_i - \overline{X})$ since fluctuations can have either sign. Note the useful identity:

$$\overline{(X - \overline{X})^2} = \overline{X^2 - 2X\overline{X} + (\overline{X})^2} = \overline{X^2} - 2\overline{X}\,\overline{X} + (\overline{X})^2 = \overline{X^2} - (\overline{X})^2$$

We also define the root-mean-square (RMS) deviation (or standard deviation):

$$\Delta X_{rms} = \sigma_X = \sqrt{\overline{(X - \overline{X})^2}} = \sqrt{\overline{X^2} - (\overline{X})^2}$$

Example: Binomial Distribution Properties (results to be shown in discussion section/homework)

- Average # of steps to the right: $\overline{n_1} = N \times p$
  (= (total # of steps) $\times$ (prob. of step right))
- Variance: $\mathrm{Var}(n_1) = \overline{n_1^2} - (\overline{n_1})^2 = N \times pq$
- RMS deviation: $\Delta n_{1,rms} = \sqrt{Npq}$
- The relative width is:
$$\frac{\Delta n_{1,rms}}{\overline{n_1}} = \frac{\sqrt{Npq}}{Np} = \sqrt{\frac{q}{p}} \times \frac{1}{\sqrt{N}}$$
- This shows the distribution becomes sharply peaked (relative width $\to 0$) when $N \gg 1$.

Physics 415 - Lecture 2

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Summary: Binomial Distribution

The binomial distribution gives the likelihood that an event with probability p occurs n times in N independent trials:

$$P_N(n) = \binom{N}{n} p^n q^{N-n} = \frac{N!}{n!(N-n)!} p^n (1-p)^{N-n}$$

where $q = 1 - p$.

- Mean: $\overline{n} = Np$
- Variance: $\sigma_n^2 = \overline{n^2} - (\overline{n})^2 = Npq$
- Relative width (RMS deviation / mean): $\frac{\Delta n_{rms}}{\overline{n}} = \frac{\sqrt{Npq}}{Np} = \sqrt{\frac{q}{p}} \frac{1}{\sqrt{N}}$

Important regime to understand is $N \gg 1$.

Gaussian Approximation to Binomial Distribution ($N \gg 1$)

It is convenient to work with $\ln P_N(n)$:

$$\ln P_N(n) = \ln N! - \ln n! - \ln(N-n)! + n \ln p + (N-n) \ln q$$

For $N \gg 1$, we use Stirling's formula (see Reif App. A.6 for derivation):

$$N! \approx \sqrt{2\pi N} \left(\frac{N}{e}\right)^N \quad (N \gg 1)$$

or more conveniently for logarithms:

$$\ln N! \approx N \ln N - N + \frac{1}{2} \ln(2\pi N)$$

Applying this to $\ln N!$, $\ln n!$, and $\ln(N-n)!$ (assuming $n \gg 1$ and $N - n \gg 1$):

$$\begin{aligned} \ln P_N(n) \approx & \left(N \ln N - N + \tfrac{1}{2} \ln(2\pi N)\right) \\ & - \left(n \ln n - n + \tfrac{1}{2} \ln(2\pi n)\right) \\ & - \left((N-n) \ln(N-n) - (N-n) + \tfrac{1}{2} \ln(2\pi(N-n))\right) \\ & + n \ln p + (N-n) \ln q \end{aligned}$$

Grouping terms:

$$\ln P_N(n) \approx \tfrac{1}{2} \ln\left(\frac{2\pi N}{2\pi n \cdot 2\pi(N-n)}\right) + N \ln N - n \ln n - (N-n) \ln(N-n) + n \ln p + (N-n) \ln q$$

Let $x = n/N$. Then $n = Nx$ and $N - n = N(1-x)$.

$$\begin{aligned}\ln P_N(n) \approx & \tfrac{1}{2}\ln\left(\frac{N}{2\pi n(N-n)}\right) \\ & + N\ln N - Nx\ln(Nx) - N(1-x)\ln(N(1-x)) \\ & + Nx\ln p + N(1-x)\ln q\end{aligned}$$

$$\begin{aligned}\ln P_N(n) \approx & \tfrac{1}{2}\ln\left(\frac{N}{2\pi n(N-n)}\right) \\ & + N\ln N - Nx(\ln N + \ln x) - N(1-x)(\ln N + \ln(1-x)) \\ & + Nx\ln p + N(1-x)\ln q\end{aligned}$$

$$\begin{aligned}\ln P_N(n) \approx & \tfrac{1}{2}\ln\left(\frac{N}{2\pi n(N-n)}\right) \\ & + (N - Nx - N(1-x))\ln N \\ & - N[x\ln x + (1-x)\ln(1-x)] \\ & + N[x\ln p + (1-x)\ln q]\end{aligned}$$

The $\ln N$ terms cancel. Let $f(x) = [x\ln x + (1-x)\ln(1-x)] - [x\ln p + (1-x)\ln q]$. Then $\ln P_N(n) \approx \frac{1}{2}\ln\left[\frac{N}{2\pi n(N-n)}\right] - Nf(n/N)$.

$$\implies P_N(n) \approx \sqrt{\frac{N}{2\pi n(N-n)}}e^{-Nf(n/N)} \quad (\text{for } n \gg 1, N-n \gg 1)$$

For N large, $P_N(n)$ will be sharply peaked near its maximum at $n = \tilde{n}$. We seek an approximation for $P_N(n)$ near $n = \tilde{n}$.

The maximum of $P_N(n)$ corresponds to the minimum of $f(x)$. We find the minimum by setting $f'(x) = \frac{\mathrm{d}f}{\mathrm{d}x} = 0$.

$$f'(x) = [\ln x + 1 - \ln(1-x) - 1] - [\ln p - \ln q] = \ln\left(\frac{x}{1-x}\right) - \ln\left(\frac{p}{q}\right) = \ln\left(\frac{qx}{p(1-x)}\right)$$

Setting $f'(\tilde{x}) = 0 \implies \frac{q\tilde{x}}{p(1-\tilde{x})} = 1 \implies q\tilde{x} = p(1-\tilde{x}) \implies (q+p)\tilde{x} = p \implies \tilde{x} = p$. So the peak occurs at $\tilde{x} = \tilde{n}/N = p \implies \tilde{n} = Np$, which is the mean value.

Now expand $f(x)$ about $x = \tilde{x} = p$:

$$f(x) \approx f(\tilde{x}) + f'(\tilde{x})(x-\tilde{x}) + \frac{1}{2}f''(\tilde{x})(x-\tilde{x})^2$$

We have $f'(\tilde{x}) = 0$.

$$f(\tilde{x}) = p\ln p + q\ln q - (p\ln p + q\ln q) = 0$$

We need the second derivative:

$$f''(x) = \frac{\mathrm{d}}{\mathrm{d}x}\ln\left(\frac{qx}{p(1-x)}\right) = \frac{p(1-x)}{qx}\cdot\frac{qp(1-x) - qx(-p)}{(p(1-x))^2} = \frac{p(1-x)}{qx}\frac{pq}{(p(1-x))^2} = \frac{q}{x(1-x)p}$$

$$f''(x) = \frac{\mathrm{d}}{\mathrm{d}x}(\ln x - \ln(1-x) - (\ln p - \ln q)) = \frac{1}{x} - \frac{1}{1-x}(-1) = \frac{1}{x} + \frac{1}{1-x} = \frac{1}{x(1-x)}$$

At $x = \tilde{x} = p$: $f''(p) = \frac{1}{p(1-p)} = \frac{1}{pq}$.

So, $f(x) \approx \frac{1}{2}f''(p)(x-p)^2 = \frac{1}{2pq}(n/N-p)^2 = \frac{(n-Np)^2}{2N^2pq}$. The exponent becomes $-Nf(n/N) \approx -N\frac{(n-Np)^2}{2N^2pq} = -\frac{(n-Np)^2}{2Npq}$.

$$\implies P_N(n) \approx \sqrt{\frac{N}{2\pi n(N-n)}}e^{-\frac{(n-Np)^2}{2Npq}}$$

Finally, because the exponential factor is sharply peaked at $n = \tilde{n} = Np$, we may approximate the n dependence in the prefactor by replacing n with $\tilde{n} = Np$ and $N - n$ with $N - \tilde{n} = Nq$:

$$n(N-n) \approx (Np)(Nq) = N^2pq$$

$$\sqrt{\frac{N}{2\pi n(N-n)}} \approx \sqrt{\frac{N}{2\pi N^2pq}} = \sqrt{\frac{1}{2\pi Npq}} = \frac{1}{\sqrt{2\pi\sigma_n^2}}$$

where $\sigma_n^2 = Npq$ is the variance. Thus, the Gaussian approximation to the binomial distribution for $N \gg 1$ is:

$$P_N(n) \approx \frac{1}{\sqrt{2\pi Npq}}e^{-\frac{(n-Np)^2}{2Npq}}$$

This can be written as:

$$P_N(n) \approx \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{(n-\mu)^2}{2\sigma^2}}$$

where $\mu = Np$ (mean) and $\sigma^2 = Npq$ (variance). This is the Gaussian (or Normal) distribution. This result is an example of the "central limit theorem".

The Gaussian distribution can be shown to be properly normalized when treated as a continuous distribution (replacing sum by integral for large N):

$$\sum_{n=0}^{N} P_N(n) \approx \int_{-\infty}^{\infty} \mathrm{d}n P_N(n) = \int_{-\infty}^{\infty} \mathrm{d}n \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{(n-\mu)^2}{2\sigma^2}} = 1$$

(See Section 1 of notes for Gaussian integrals).

Distributions with Multiple Variables

Consider two random variables u and v (generalization to more variables is straightforward).

- Possible values: $\{u_i\}, i = 1, \ldots, M$; $\{v_j\}, j = 1, \ldots, L$.
- Joint probability: $P(u_i, v_j)$ = prob that $u = u_i$ and $v = v_j$.
- Normalization: $\sum_{i=1}^{M}\sum_{j=1}^{L} P(u_i, v_j) = 1$.
- "Unconditional" probability distributions (marginal distributions):
  - $P_u(u_i) = \sum_{j=1}^{L} P(u_i, v_j)$ = prob $u = u_i$, irrespective of v.
  - $P_v(v_j) = \sum_{i=1}^{M} P(u_i, v_j)$ = prob $v = v_j$, irrespective of u.

Statistical Independence

An important special case is when the probability that one variable assumes a certain value is independent of the value assumed by the other variable. The variables are "statistically independent" or "uncorrelated". In this case:

$$P(u_i, v_j) = P_u(u_i)P_v(v_j) \quad \text{(for statistically independent } u, v\text{)}$$

Mean Values

The mean of a function $F(u,v)$ is:

$$\overline{F(u,v)} = \sum_{i=1}^{M} \sum_{j=1}^{L} P(u_i,v_j) F(u_i,v_j)$$

A special case is the mean of a product $f(u) \times g(v)$ when u and v are statistically independent:

$$\begin{aligned}
\overline{f(u)g(v)} &= \sum_{i,j} P(u_i,v_j) f(u_i) g(v_j) \\
&= \sum_{i,j} P_u(u_i) P_v(v_j) f(u_i) g(v_j) \quad \text{(using independence)} \\
&= \left(\sum_{i=1}^{M} P_u(u_i) f(u_i) \right) \times \left(\sum_{j=1}^{L} P_v(v_j) g(v_j) \right) \\
&= \overline{f(u)} \times \overline{g(v)}
\end{aligned}$$

$$\implies \overline{f(u)g(v)} = \overline{f(u)} \times \overline{g(v)} \quad \text{if } u, v \text{ are statistically independent}$$

The average "factorizes". (This is not true in general!)

Continuous Probability Distributions

We will often encounter "continuous" probability distributions, where a random variable X can assume a continuous range of values, e.g., $a_1 < x < a_2$. Example: Gaussian distribution $\mathcal{P}(()x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$ for $-\infty < x < \infty$.

For a continuous distribution, it does not make sense to consider the probability of X taking any particular value (which would be vanishingly small). Rather, we consider the probability that the random variable lies in a small range between x and $x + \mathrm{d}x$.

- $\mathcal{P}(()x)\mathrm{d}x$ = probability to find the random variable in the range $(x, x + \mathrm{d}x)$.
- $\mathcal{P}(()x)$ is the "probability density".
- Normalization: $\int_{a_1}^{a_2} \mathrm{d}x \mathcal{P}(()x) = 1$. (cf. $\sum P(x_i) = 1$)
- Mean of a function $f(x)$: $\overline{f(x)} = \int_{a_1}^{a_2} \mathrm{d}x \mathcal{P}(()x) f(x)$. (cf. $\overline{f(x)} = \sum P(x_i) f(x_i)$)

Examples of important continuous probability distributions:

- Gaussian: $\mathcal{P}(()x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/(2\sigma^2)}$
- Dirac delta: $\mathcal{P}(()x) = \delta(x - x_0)$
- Lorentzian: $\mathcal{P}(()x) = \frac{1}{\pi} \frac{\gamma}{\gamma^2 + (x - x_0)^2}$

Transformation of Continuous Distributions

For continuous probability distributions, it's important to know how to transform from one random variable x to another random variable $y = f(x)$. That is, given the distribution $\mathcal{P}()x(x)$, what is the distribution $\mathcal{P}()y(y)$ of $y = f(x)$?

Consider the probability conservation: the probability that y falls in the range $(y, y + \mathrm{d}y)$ must be equal to the probability that x falls in the corresponding range(s) $(x_i, x_i + \mathrm{d}x_i)$. In general, there may be multiple points x_i such that $y = f(x_i)$.

From the diagram: $\mathcal{P}(_{)}y(y)|\mathrm{d}y| = \sum_i \mathcal{P}(_{)}x(x_i)|\mathrm{d}x_i|$, where the sum is over all x_i such that $f(x_i) = y$. Since $\mathrm{d}y = \frac{\mathrm{d}f}{\mathrm{d}x}\mathrm{d}x = f'(x)\mathrm{d}x$, we have $|\mathrm{d}x_i| = \frac{|\mathrm{d}y|}{|f'(x_i)|} = |\frac{dx}{dy}|_{x=x_i}|\mathrm{d}y|$.

$$\mathcal{P}(_{)}y(y)|\mathrm{d}y| = \sum_i \mathcal{P}(_{)}x(x_i)\left|\frac{dx}{dy}\right|_{x=x_i}|\mathrm{d}y|$$

$$\implies \mathcal{P}(_{)}y(y) = \sum_i \mathcal{P}(_{)}x(x_i)\left|\frac{dx}{dy}\right|_{x=x_i}$$

where the sum is over all roots x_i of $y = f(x)$ for a fixed y.

Example: X-component of a Random 2D Vector

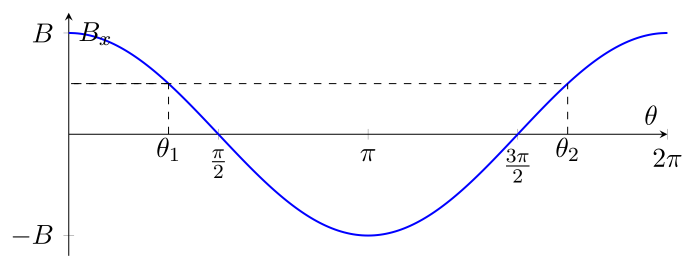
Consider a 2D vector $\vec{B}$ with fixed length $B = |\vec{B}|$, equally likely to point in any direction θ (where θ is the angle with the x-axis). The probability distribution for the angle θ is uniform:

$$\mathcal{P}(_{)}\theta(\theta) = \frac{1}{2\pi}, \quad 0 \le \theta < 2\pi$$

Let $y = B_x$ be the x-component of $\vec{B}$. We have the relation:

$$B_x(\theta) = B\cos\theta$$

We want to find the probability distribution $\mathcal{P}(_{)}B_x(B_x)$. Note that $-B \le B_x \le B$.



For a given value of B_x (where $-B < B_x < B$), there are two angles θ_1 and $\theta_2 = 2\pi - \theta_1$ such that $B_x = B\cos\theta_1 = B\cos\theta_2$. (Let $\theta_1 = \arccos(B_x/B)$). We use the general formula: $\mathcal{P}(_{)}B_x(B_x) = \sum_{i=1,2}\mathcal{P}(_{)}\theta(\theta_i)\left|\frac{\mathrm{d}\theta}{\mathrm{d}B_x}\right|_{\theta=\theta_i}$. We need the derivative $\frac{\mathrm{d}\theta}{\mathrm{d}B_x}$. It's easier to compute $\frac{\mathrm{d}B_x}{\mathrm{d}\theta}$:

$$\frac{\mathrm{d}B_x}{\mathrm{d}\theta} = \frac{\mathrm{d}}{\mathrm{d}\theta}(B\cos\theta) = -B\sin\theta$$

So, $\left|\frac{\mathrm{d}\theta}{\mathrm{d}B_x}\right| = \frac{1}{|-B\sin\theta|} = \frac{1}{B|\sin\theta|}$. Since $\sin^2\theta + \cos^2\theta = 1$, $|\sin\theta| = \sqrt{1-\cos^2\theta} = \sqrt{1-(B_x/B)^2} = \frac{\sqrt{B^2-B_x^2}}{B}$. Therefore, $\left|\frac{\mathrm{d}\theta}{\mathrm{d}B_x}\right| = \frac{1}{B(\sqrt{B^2-B_x^2}/B)} = \frac{1}{\sqrt{B^2-B_x^2}}$. This derivative is the same for θ_1 and θ_2 since $|\sin(\theta_1)| = |\sin(2\pi-\theta_1)|$.

Now apply the formula:

$$\begin{aligned}
\mathcal{P}(_{)}B_x(B_x) &= \mathcal{P}(_{)}\theta(\theta_1)\left|\frac{\mathrm{d}\theta}{\mathrm{d}B_x}\right|_{\theta_1} + \mathcal{P}(_{)}\theta(\theta_2)\left|\frac{\mathrm{d}\theta}{\mathrm{d}B_x}\right|_{\theta_2} \\
&= \left(\frac{1}{2\pi}\right)\frac{1}{\sqrt{B^2-B_x^2}} + \left(\frac{1}{2\pi}\right)\frac{1}{\sqrt{B^2-B_x^2}} \\
&= 2\times\frac{1}{2\pi}\frac{1}{\sqrt{B^2-B_x^2}}
\end{aligned}$$

$$\mathcal{P}(_)B_x(B_x) = \frac{1}{\pi\sqrt{B^2 - B_x^2}} \quad \text{for } -B < B_x < B$$

This distribution is peaked near $B_x = \pm B$ and minimum at $B_x = 0$.