Iván Mauricio Burbano Aldana

Perimeter Scholars International

Statistical Mechanics

Homework 1: Gaussian Ising and Polya's Problem

1.a) a) $$\int dx\, e^{-\omega^2 x^2} = \frac{1}{|\omega|}\int dx\, e^{-x^2} = \frac{1}{|\omega|}\left(\int dx\, e^{-x^2}\int dy\, e^{-y^2}\right)^{1/2}$$

$$= \frac{1}{|\omega|}\left(\int dx\, dy\, e^{-(x^2+y^2)}\right)^{1/2} = \frac{1}{|\omega|}\left(\int_0^{2\pi} d\theta \int_0^{\infty} dr\, r\, e^{-r^2}\right)^{1/2}$$

$$= \frac{\sqrt{2\pi}}{|\omega|}\left(\left[-\frac{1}{2}e^{-r^2}\right]_0^{\infty}\right)^{1/2} = \frac{\sqrt{2\pi}}{|\omega|}\cancel{\sqrt{\frac{1}{2}}} = \frac{\sqrt{\pi}}{|\omega|}$$

b) $$\int dx\, e^{-\omega^2 x^2 + jx} = \int dx\, e^{-\omega^2 (x - j/2\omega^2)^2 + \frac{j^2}{4\omega^2}}$$

$$= \int dx\, e^{-\omega^2 x^2}\, e^{j^2/4\omega^2} = \frac{\sqrt{\pi}}{|\omega|}\, e^{j^2/4\omega^2}$$

c) We have

$$\int dx\, e^{-\omega^2 x^2} x^n = \int dx \frac{d^n}{dj^n} e^{-\omega^2 x^2 + jx}\Big|_{j=0}$$

$$= \frac{d^n}{dj^n} \int dx\, e^{-\omega^2 x^2 + jx}\Big|_{j=0} = \frac{\sqrt{\pi}}{|\omega|} \frac{d^n}{dj^n}\left(e^{j^2/4\omega^2}\right)\Big|_{j=0}$$

$$= \frac{\sqrt{\pi}}{|\omega|} \sum_{m=0}^{\infty} \frac{1}{m!}\left(\frac{1}{4\omega^2}\right)^m \frac{d^n}{dj^n} j^{2m}\Big|_{j=0}$$

$$= \frac{\sqrt{\pi}}{|\omega|} \sum_{m=0}^{\infty} \frac{1}{m!}\left(\frac{1}{4\omega^2}\right)^m \delta_{n,2m}\,(2m)!$$

$$= \begin{cases} 0, & n \in 2\mathbb{N}+1 \\ \frac{\sqrt{\pi}}{|\omega|}\left(\frac{1}{4\omega^2}\right)^{n/2} \frac{n!}{(n/2)!} = \frac{\sqrt{\pi}}{|\omega|}\frac{2^{n/2}}{(2|\omega|)^n}\frac{n!}{2^{n/2}(n/2)!} & \end{cases}$$

$$= \frac{\sqrt{\pi}}{2^{n/2}|\omega|^{n+1}} \frac{\cancel{n}(n-1)\cancel{(n-2)}(n-3)\cancel{\cdots}}{\cancel{n}\cancel{(n-2)}\cancel{(n-4)}\cdots} \frac{1}{2}$$

$$= \frac{\sqrt{\pi}}{|\omega|} \frac{(n-1)!!}{(2\omega^2)^{n/2}}, \qquad n \in 2\mathbb{N}^+$$

Another way of deriving this, is by finding an operator Q so that

$$\int dx\, e^{-\omega^2 x^2} Q f(x) = \int dx \frac{d}{dx}\left(e^{-\omega^2 x^2} f(x)\right) = 0,$$

i.e. with domain $f \in C^\infty(\mathbb{R})$ s.t.

$$\left[e^{-\omega^2 x^2} f(x) \right]_{x=-\infty}^{\infty} = 0.$$

We have

$$\frac{d}{dx}\left(e^{-\omega^2 x^2} f(x) \right) = -2\omega^2 x\, e^{-\omega^2 x^2} f(x) + e^{-\omega^2 x^2} f'(x)$$

$$= e^{-\omega^2 x^2} \left(f'(x) - 2\omega^2 x f(x) \right).$$

We thus define

$$Qf(x) = f'(x) - 2\omega^2 x f(x).$$

We then get

$$Q_x x^n = n x^{n-1} - 2\omega^2 x^{n+1}.$$

Since elements in the image of Q have integral 0 w.r.t. the measure $dx\, e^{-\omega^2 x^2}$, we conclude

$$\int dx\, e^{-\omega^2 x^2} x^{n+1} = \frac{n}{2\omega^2} \int dx\, e^{-\omega^2 x^2} x^{n-1}.$$

Thus

$$\int dx\, e^{-\omega^2 x^2} x^{2n} = \frac{2n-1}{2\omega^2} \int dx\, e^{-\omega^2 x^2} x^{2(n-1)}$$

Thus, the claim

$$\int dx\, e^{-\omega^2 x^2} x^{2n} = \frac{\sqrt{\pi}}{|\omega|} \frac{(2n-1)!!}{(2\omega^2)^n}$$

can be proved by induction. In the case

$n=1$,

$$\int dx\, e^{-\omega^2 x^2} x^2 = -\frac{\partial}{\partial \omega^2} \int dx\, e^{-\omega^2 x^2}$$

$$= -\frac{\partial}{\partial \omega^2} \sqrt{\frac{\pi}{\omega^2}} = +\sqrt{\pi} \left(+\frac{1}{2}\right) (\omega^2)^{-3/2}$$

$$= \frac{\sqrt{\pi}}{|\omega|} \frac{1}{2\omega^2},$$

If we assume it is true for $n-1$

we then have

$$\int dx\, e^{-\omega^2 x^2} x^{2n} = \frac{2n-1}{2\omega^2} \frac{\sqrt{\pi}}{|\omega|} \frac{(2n-3)!!}{(2\omega^2)^{n-1}}$$

$$= \frac{\sqrt{\pi}}{|\omega|} \frac{(2n-1)!!}{(2\omega^2)^n}.$$

d) Since $\vec{x}\cdot\Omega\vec{x} = x^i\Omega_{ij}x^j = x^i\Omega_{(ij)}x^j$, we may assume Ω is symmetric. By the spectral theorem, there exists $T \in O(n)$ s.t.

$$T^T\Omega T = D = \mathrm{diag}(d_1, \ldots, d_n)$$

Then, under the change of coordinates T, we have a Jacobian $DT = T$, with determinant $|T| = 1$. Thus

$$\int d^n\vec{x}\, e^{-\vec{x}\cdot\Omega\vec{x}} = \int d^n\vec{x}\, e^{-\vec{x}\cdot T^T D T\vec{x}}$$

$$= \int d^n\vec{x}\, e^{-T\vec{x}\cdot D T\vec{x}}$$

$$= \int d^n\vec{x}\, e^{-\vec{x}\cdot D\vec{x}} = \int d^n\vec{x}\, e^{-\sum_{i=1}^{n} d_i(x_i)^2}$$

$$= \int d^n\vec{x} \prod_{i=1}^{n} e^{-d_i x_i^2} = \prod_{i=1}^{n}\int dx_i\, e^{-d_i x_i^2}$$

$$= \prod_{i=1}^{n}\sqrt{\frac{\pi}{d_i}} = \frac{\pi^{n/2}}{\sqrt{\prod_{i=1}^{n} d_i}} = \frac{\pi^{n/2}}{\sqrt{\det D}}$$

$$= \frac{\pi^{n/2}}{\sqrt{\det \Omega}} .$$

Remark: Strictly speaking, this only follows from our previous expression if Ω is positive definite. It is in this case that $d_1, \ldots, d_n \in (0,\infty)$.

c) Observe that, since Ω is positive definite and thus invertible

$$-\left(\vec{x} - \tfrac{1}{2}\Omega^{-1}\vec{J}\right)\cdot\Omega\left(\vec{x} - \tfrac{1}{2}\Omega^{-1}\vec{J}\right) = -\vec{x}\cdot\Omega\vec{x} + \tfrac{1}{2}\Omega^{-1}\vec{J}\cdot\Omega\vec{x}$$
$$+ \vec{x}\cdot\tfrac{1}{2}\cancel{\Omega\Omega^{-1}}\vec{J} - \tfrac{1}{4}\Omega^{-1}\vec{J}\cdot\cancel{\Omega\Omega^{-1}}\vec{J}$$

$$= -\vec{x}\cdot\Omega\vec{x} + \tfrac{1}{2}\vec{J}\cdot\cancel{\Omega^{-1}\Omega}\vec{x} + \tfrac{1}{2}\vec{x}\cdot\vec{J} - \tfrac{1}{4}\vec{J}\cdot\Omega^{-1}\vec{J}$$

$$= -\vec{x}\cdot\Omega\vec{x} + \vec{J}\cdot\vec{x} - \tfrac{1}{4}\vec{J}\cdot\Omega^{-1}\vec{J}.$$

Thus

$$\int d^n\vec{x}\, e^{-\vec{x}\cdot\Omega\vec{x} + \vec{J}\cdot\vec{x}} = \int d^n\vec{x}\, e^{-\left(\vec{x} - \frac{1}{2}\Omega^{-1}\vec{J}\right)\cdot\Omega\left(\vec{x} - \frac{1}{2}\Omega^{-1}\vec{J}\right) + \frac{1}{4}\vec{J}\cdot\Omega^{-1}\vec{J}}$$

$$= e^{\frac{1}{4}\vec{J}\cdot\Omega^{-1}\vec{J}} \int d^n\vec{x}\, e^{-\vec{x}\cdot\Omega\vec{x}} = \frac{\pi^{n/2}}{\sqrt{\det\Omega}}\, e^{\frac{1}{4}\vec{J}\cdot\Omega^{-1}\vec{J}} .$$

f) $$\int d^n\vec{x}\, e^{-\vec{x}\cdot\Omega\vec{x}} x^a x^b = \frac{\partial^2}{\partial J_a \partial J_b} \int d^n\vec{x}\, e^{-\vec{x}\cdot\Omega\vec{x} + \vec{J}\cdot\vec{x}} \Big|_{\vec{J}=\vec{0}}$$

$$= \frac{\pi^{n/2}}{\sqrt{\det\Omega}} \frac{\partial^2}{\partial J_a \partial J_b} e^{\frac{1}{4} J_c (\Omega^{-1})^{cd} J_d} \Big|_{\vec{J}=\vec{0}}$$

$$= \frac{\pi^{n/2}}{\sqrt{\det\Omega}} \frac{\partial^2}{\partial J_a \partial J_b} \left(1 + \frac{1}{4} J_c (\Omega^{-1})^{cd} J_d + \mathcal{O}(\|\vec{J}\|^4) \right) \Big|_{\vec{J}=\vec{0}}$$

$$= \frac{\pi^{n/2}}{\sqrt{\det\Omega}} \frac{1}{4} \frac{\partial}{\partial J_a} \left(\delta^b_c (\Omega^{-1})^{cd} J_d + J_c (\Omega^{-1})^{cd} \delta^b_d \right) \Big|_{\vec{J}=\vec{0}}$$

$$= \frac{\pi^{n/2}}{\sqrt{\det\Omega}} \frac{1}{4} \left((\Omega^{-1})^{bd} \delta^a_d + \delta^a_c (\Omega^{-1})^{cb} \right) \Big|_{\vec{J}=\vec{0}}$$

$$= \frac{\pi^{n/2}}{\sqrt{\det\Omega}} \frac{1}{4} \left((\Omega^{-1})^{ba} + (\Omega^{-1})^{ab} \right)$$

$$= \frac{\pi^{n/2}}{\sqrt{\det\Omega}} \frac{(\Omega^{-1})^{ab}}{2} .$$

Thus

$$\langle x_a x_b \rangle = \frac{(\Omega^{-1})^{ab}}{2} .$$

b) We can adapt our result to

$$\int d^n\vec{x}\, e^{-\frac{1}{2}\vec{x}\cdot\Omega\vec{x} + \vec{J}\cdot\vec{x}} = \frac{\pi^{n/2}}{\sqrt{\det\left(\frac{\Omega}{2}\right)}} e^{\frac{1}{4}\vec{J}\cdot\left(\frac{\Omega}{2}\right)^{-1}\vec{J}}$$

$$= \frac{(2\pi)^{n/2}}{\sqrt{\det \Omega}} \quad e^{\frac{1}{2}\vec{J}\cdot\Omega^{-1}\vec{J}} .$$

Thus

$$\int d^n\vec{x}\; x^{i_1}\cdots x^{i_k}\, e^{-\frac{1}{2}\vec{x}\cdot\Omega\vec{x}} = \frac{\partial}{\partial J_{i_1}} \cdots \frac{\partial}{\partial J_{i_m}} \int d^n\vec{x}\, e^{-\frac{1}{2}\vec{x}\cdot\Omega\vec{x} + \vec{J}\cdot\vec{x}} \Big|_{\vec{J}=\vec{0}}$$

$$= \frac{(2\pi)^{n/2}}{\sqrt{\det\Omega}} \left(\prod_{m=1}^{k} \frac{\partial}{\partial J_{i_m}} \right) e^{\frac{1}{2}\vec{J}\cdot\Omega^{-1}\vec{J}} \Big|_{\vec{J}=\vec{0}}$$

$$= \frac{(2\pi)^{n/2}}{\sqrt{\det\Omega}} \sum_{r=0}^{\infty} \frac{1}{r!} \prod_{m=1}^{k} \frac{\partial}{\partial J_{i_m}} \left(\frac{1}{2}\vec{J}\cdot\Omega^{-1}\vec{J} \right)^r \Big|_{\vec{J}=\vec{0}} .$$

This is clearly null when k is odd. Thus, we take $k = 2p$ and

$$\langle x^{i_1}\cdots x^{i_{2p}} \rangle = \sum_{r=0}^{\infty} \frac{1}{r!} \left(\prod_{m=1}^{2p} \frac{\partial}{\partial J_{i_m}} \right) \left(\frac{1}{2^r} J_{j_1}(\Omega^{-1})^{j_1 l_1} J_{l_1} \cdots J_{j_r}(\Omega^{-1})^{j_r l_r} J_{l_r} \right)$$

$$= \frac{1}{2^p p!} \prod_{k=1}^{2p} (\Omega^{-1})^{j_k l_k} \prod_{m=1}^{2p} \frac{\partial}{\partial J_{i_m}} \left(J_{j_1} J_{l_1} \cdots J_{j_p} J_{l_p} \right) \Big|_{\vec{J}=\vec{0}}.$$

Now, the derivative is null unless $j_1, l_1, \ldots, j_p, l_p$ and $i_1, \ldots, i_{2p}$ agree as a multiset. Thus, the multisets $(j_1,l_1),\dots,(j_p,l_p)$ have to be pairings of the list $(i_1,\dots,i_{2p})$. These pairings are invariant under the exchange $j_r \leftrightarrow l_r$, introducing a multiplicity of 2^p on every term. Moreover, the exchanges $(j_r,l_r) \longleftrightarrow (j_{r'},l_{r'})$ also leave the pairings invariant. This introduces a multiplicity of $p!$. Both of these cancel the denominator and we have

$$\langle x^{i_1}\cdots x^{i_{2p}}\rangle = \sum_{\substack{\text{Pairings } P \\ \text{of } i_1,\dots,i_{2p}}} \prod_{(a,b)\in P} (\Omega^{-1})^{ab}.$$

A more rigorous approach is based on the second solution we gave to c). We thus want to find a new operator Q s.t

$$e^{-\frac{1}{2}\vec{x}\cdot\Omega\vec{x}}\, Q\vec{F}(\vec{x}) = \mathrm{Div}\left(e^{-\frac{1}{2}\vec{x}\cdot\Omega\vec{x}}\, F(\vec{x})\right)$$

$$= e^{-\frac{1}{2}\vec{x}\cdot\Omega\vec{x}}\left(-\frac{1}{2}\left(\delta^j_i\,\Omega_{jk}x^k + x^j\Omega_{jk}\delta^k_i\right)F^i(\vec{x}) + \vec{\nabla}\cdot\vec{F}(\vec{x})\right)$$

$$= e^{-\frac{1}{2}\vec{x}\cdot\Omega\vec{x}} \left(\vec{\nabla}\cdot\vec{F}(\vec{x}) - \vec{x}\cdot\Omega\,\vec{F}(\vec{x}) \right),$$

i.e.

$$Q\vec{F}(\vec{x}) = \vec{\nabla}\cdot\vec{F}(\vec{x}) - \vec{x}\cdot\Omega\vec{F}(\vec{x}).$$

Moreover, if $\vec{F}$ is nice enough (e.g. a vector field with polynomial coefficients)

$$\int d^n\vec{x}\, e^{-\frac{1}{2}\vec{x}\cdot\Omega\vec{x}}\, Q\vec{F}(\vec{x}) = \int d^n\vec{x}\, \mathrm{Div}\left(e^{-\frac{1}{2}\vec{x}\cdot\Omega\vec{x}}\,\vec{F}(\vec{x})\right) = 0$$

Consider

$$\vec{F}(\vec{x}) = x^{i_1}\cdots x^{i_m}\frac{\partial}{\partial x^t}$$

Thus

$$Q\vec{F}(\vec{x}) = \sum_{r=1}^{m} x^{i_1}\cdots\hat{x}^{i_r}\cdots x^{i_m}\,\delta^{i_r}{}_t - x^j\Omega_{jt}\,x^{i_1}\cdots x^{i_m}.$$

From the above considerations we conclude

$$\langle x^j x^{i_1}\cdots x^{i_m}\rangle = (\Omega^{-1})^{jt}\sum_{r=1}^{m}\langle x^{i_1}\cdots\hat{x}^{i_r}\cdots x^{i_m}\rangle\delta^{i_r}{}_t$$

$$= \sum_{r=1}^{m}(\Omega^{-1})^{j i_r}\langle x^{i_1}\cdots\hat{x}^{i_r}\cdots x^{i_m}\rangle,$$

Relabeling,

$$\langle x^{i_1} \cdots x^{i_{2p}} \rangle = \sum_{r=1}^{2p} (\Omega^{-1})^{i_{2p} i_r} \langle x^{i_1} \cdots \hat{x}^{i_r} \cdots \hat{x}^{i_{2p}} \rangle.$$

The theorem follows by induction.

c) To agree with the results of the lecture and avoid factors of 2, we will instead consider the action

$$S(s) = \frac{1}{2} \sum_{\vec{x},\vec{y} \in \mathbb{Z}^d} s(\vec{x}) A(\vec{x}-\vec{y}) s(\vec{y}).$$

For every $f \in \mathbb{R}^{\mathbb{Z}^d}$, let

$$\tilde{f}(\vec{k}) = \sum_{\vec{x} \in \mathbb{Z}^d} e^{-i\vec{k}\cdot\vec{x}} f(\vec{x}).$$

Note that

$$\tilde{f}(-\vec{k}) = \sum_{\vec{x} \in \mathbb{Z}^d} e^{i\vec{k}\cdot\vec{x}} f(\vec{x}) = \tilde{f}(\vec{k})^*$$

and

$$\int_{[-\pi,\pi]^d} \frac{d^d\vec{k}}{(2\pi)^d} e^{i\vec{k}\cdot\vec{x}} \tilde{f}(\vec{k}) = \sum_{\vec{y} \in \mathbb{Z}^d} \int_{[-\pi,\pi]^d} \frac{d^d\vec{k}}{(2\pi)^d} e^{i\vec{k}\cdot(\vec{x}-\vec{y})} f(\vec{y})$$

$$= \sum_{\vec{y} \in \mathbb{Z}^d} \delta_{\vec{x},\vec{y}} f(\vec{y}) = f(\vec{x}).$$

Thus

$$\frac{1}{2}\sum_{\vec{x},\vec{y}\in\mathbb{Z}^d} s(\vec{x})\,A(\vec{x}-\vec{y})\,s(\vec{y}) = \frac{1}{2}\int_{[-\pi,\pi]^{2d}} \frac{d^d\vec{k}\,d^d\vec{k}'}{(2\pi)^d(2\pi)^d} \sum_{\vec{x},\vec{y}\in\mathbb{Z}^d} e^{i\vec{k}\cdot\vec{x}+i\vec{k}'\cdot\vec{y}}\,A(\vec{x}-\vec{y})\,\tilde{s}(\vec{k})\tilde{s}(\vec{k}')$$

$$= \frac{1}{2}\int_{[-\pi,\pi]^{2d}} \frac{d^d\vec{k}\,d^d\vec{k}'}{(2\pi)^d(2\pi)^d} \sum_{\vec{x},\vec{y}\in\mathbb{Z}^d} e^{i(\vec{x}+\vec{y})\cdot\frac{\vec{k}+\vec{k}'}{2}+i(\vec{x}-\vec{y})\cdot\frac{\vec{k}-\vec{k}'}{2}}\,A(\vec{x}-\vec{y})\,\tilde{s}(\vec{k})\,\tilde{s}(\vec{k}')$$

$$= \frac{1}{2}\int_{[-\pi,\pi]^{2d}} \frac{d^d\vec{k}\,d^d\vec{k}'}{(2\pi)^d}\,\delta\left(\frac{\vec{k}+\vec{k}'}{2}\right)\tilde{s}(\vec{k})\tilde{s}(\vec{k}') \sum_{\vec{r}\in\mathbb{Z}^d} e^{i\vec{r}\cdot\frac{\vec{k}-\vec{k}'}{2}}\,A(\vec{r})$$

$$= \cancel{\frac{2}{2}}\int_{[-\pi,\pi]^d} \frac{d^d\vec{k}}{(2\pi)^d}\,|\tilde{s}(\vec{k})|^2 \sum_{\vec{r}\in\mathbb{Z}^d} e^{i\vec{r}\cdot\vec{k}}\,A(\vec{r})$$

$$= \int_{[-\pi,\pi]^d} \frac{d^d\vec{k}}{(2\pi)^d}\,\hat{A}(\vec{k})\,|\hat{s}(\vec{k})|^2,$$

where

$$\hat{A}(\vec{k}) := \sum_{\vec{r}\in\mathbb{Z}^d} e^{i\vec{r}\cdot\vec{k}}\,A(\vec{r}).$$

We thus see that precisely $\hat{A}(\vec{k})$ corresponds to the eigenvalues of A. Since it is a continuous spectrum of eigenvalus, trying to compute $\det A$ as a product of these is very unnatural. However, using the formula

$$\det A = e^{\operatorname{tr} \ln A},$$

these products correspond to a sum which can be extended to an integral. On the other hand, the inverse of A

$$\sum_{\vec{y} \in \mathbb{Z}^d} A(\vec{x}-\vec{y})\, G(\vec{y}) = \delta_{\vec{x},\vec{0}}$$

can also be found via fourier transform.

Indeed

$$\delta_{\vec{x},\vec{0}} = \int_{[-\pi,\pi]^d} \frac{d^d\vec{k}}{(2\pi)^d} \sum_{\vec{y} \in \mathbb{Z}^d} e^{-i\vec{k}\cdot\vec{y}} A(\vec{x}-\vec{y})\, \hat{G}(\vec{k})$$

$$= \int_{[-\pi,\pi]^d} \frac{d^d\vec{k}}{(2\pi)^d}\, e^{-i\vec{k}\cdot\vec{x}} \hat{A}(\vec{k})\hat{G}(\vec{k}),$$

so that $\hat{G}(\vec{k}) = \dfrac{1}{\hat{A}(\vec{k})}$ and we conclude

$$G(\vec{x}) = \int_{[-\pi,\pi]^d} \frac{d^d\vec{k}}{(2\pi)^d}\, e^{-i\vec{k}\cdot\vec{x}} \frac{1}{\hat{A}(\vec{k})},$$

$$\sum_{\vec{x},\vec{y}\in\mathbb{Z}^d} J(\vec{x})\,G(\vec{x}-\vec{y})\,J(\vec{y}) = \int_{[-\pi,\pi]^d} \sum_{\vec{x},\vec{y}} \frac{d^d\vec{k}}{(2\pi)^d}\, e^{-i\vec{k}\cdot(\vec{x}-\vec{y})}\, J(\vec{x})\,J(\vec{y})/\hat{\Delta}(\vec{k}),$$

We conclude

$$Z = \int_{(\mathbb{R})^{\mathbb{Z}^d}} ds\; \exp\Big(-S(s) + \sum_{\vec{x}\in\mathbb{Z}^d} J(\vec{x})\cdot s(\vec{x})\Big)$$

$$= \Big(\det\Big(\frac{\Delta}{2\pi}\Big)\Big)^{-1/2} e^{\frac{1}{2}\sum_{\vec{x},\vec{y}\in\mathbb{Z}^d} J(\vec{x})G(\vec{x}-\vec{y})J(\vec{y})}$$

$$= e^{-\frac{1}{2}\int_{[-\pi,\pi]^d} \frac{d^d\vec{k}}{(2\pi)^d}\log\left(\hat{\Delta}(\vec{k})\right) + \int_{[-\pi,\pi]^d} \frac{d^d\vec{k}}{(2\pi)^d}\sum_{\vec{x},\vec{y}\in\mathbb{Z}^d} e^{-i\vec{k}\cdot(\vec{x}-\vec{y})} J(\vec{x})J(\vec{y})/\hat{\Delta}(}$$

d) We have

$$\langle s(\vec{x})s(\vec{y})\rangle = G(\vec{x}-\vec{y}).$$

e) Applying Wick's theorem

$$\langle s(\vec{x})\,s(\vec{y})\,s(\vec{w})\,s(\vec{z})\rangle = G(\vec{x}-\vec{y})\,G(\vec{w}-\vec{z}) + G(\vec{x}-\vec{w})\,G(\vec{y}-\vec{z})$$
$$+ G(\vec{x}-\vec{z})\,G(\vec{y}-\vec{w})$$

2.a) The probability for being at $\vec{r} \in \mathbb{Z}^d$ after t steps is

$$P_t(\vec{r}) = \frac{1}{(2d)^t} \sum_{\vec{v}_1 \in con_\pm} \cdots \sum_{\vec{v}_t \in con_\pm} \delta_{\vec{r}, \sum_{i=1}^{t} \vec{v}_i}$$

$$= \frac{1}{(2d)^t} \sum_{\vec{v}_1 \in con_\pm} \cdots \sum_{\vec{v}_t \in con_\pm} \int_{[-\pi,\pi]^d} \frac{d^d\vec{q}}{(2\pi)^d}\, e^{i\vec{q}\cdot(\vec{r} - \sum_{i=1}^{t} \vec{v}_i)}$$

$$= \int_{[-\pi,\pi]^d} \frac{d^d\vec{q}}{(2\pi)^d}\, e^{i\vec{q}\cdot\vec{r}} \prod_{i=1}^{t} \sum_{\vec{v}_i \in con_\pm} \frac{e^{i\vec{q}\cdot\vec{v}_i}}{2d}$$

$$= \int_{[-\pi,\pi]^d} \frac{d^d\vec{q}}{(2\pi)^d}\, e^{i\vec{q}\cdot\vec{r}} \prod_{i=1}^{t} \sum_{\mu=1}^{d} \frac{1}{d} \cos(q_\mu)$$

$$= \int_{[-\pi,\pi]^d} \frac{d^d\vec{q}}{(2\pi)^d}\, e^{i\vec{q}\cdot\vec{r}} \left(\frac{1}{d} \sum_{\mu=1}^{d} \cos(q_\mu) \right)^t,$$

where $con_\pm = \{\pm\hat{e}_1, \dots, \pm\hat{e}_d\}$. For big $\vec{r}$, the integrand is dominated for small $\vec{q}$. Thus

$$P_t(\vec{r}) = \int_{[-\pi,\pi]^d} \frac{d^d\vec{q}}{(2\pi)^d}\, e^{i\vec{q}\cdot\vec{r}} \left(1 - \frac{1}{2d} \sum_{\mu=1}^{d} q_\mu^2 + \mathcal{O}(\|\vec{q}\|^4) \right)^t$$

$$= \int_{[-\pi,\pi]^d} \frac{d^d\vec{q}}{(2\pi)^d}\, e^{i\vec{q}\cdot\vec{r}} \left(1 - \frac{t}{2d} \sum_{\mu=1}^{d} q_\mu^2 + \mathcal{O}(\|\vec{q}\|^4) \right)$$

$$= \int_{[-\pi,\pi]^d} \frac{d^d\vec{q}}{(2\pi)^d}\, e^{i\vec{q}\cdot\vec{r} - \frac{t}{2d}\vec{q}^{\,2}} + \mathcal{O}(\|\vec{q}\|^4)$$

$$\approx \int \frac{d^d\vec{q}}{(2\pi)^d}\, e^{i\vec{q}\cdot\vec{r} - \frac{t}{2d}\vec{q}^{\,2}} = \frac{1}{(2\pi)^d}\left(\frac{2\pi d}{t}\right)^{d/2} e^{-\vec{r}^{\,2}/(2t/d)}$$

$$= \left(\frac{\cancel{2}\cancel{\pi} d}{\underset{2}{\cancel{4}}\pi^{\cancel{2}} t}\right)^{d/2} e^{-\vec{r}^{\,2}/(2t/d)} = \frac{1}{t^{d/2}}\frac{1}{(2\pi\sigma_0^2)^{d/2}}\, e^{-\vec{r}^{\,2}/2\sigma_0^2 t}$$

with $\sigma_0^2 = \frac{1}{d}$. Rescalling $\vec{r}\,' = \vec{r}/\sqrt{t}$, we obtain

$$P'(\vec{r}\,') = P_t(\sqrt{t}\,\vec{r}\,') = \frac{1}{t^{d/2}}\frac{1}{(2\pi\sigma_0^2)^{d/2}}\, e^{-\frac{\vec{r}\,'^2}{2\sigma_0^2}}.$$

Observe that the variance of P is

$$\langle x^\mu x^\nu\rangle = \sum_{\vec{v}\in can_\pm} \frac{1}{2d} v^\mu v^\nu = \sum_{m\in\{\pm\}} \sum_{\lambda=1}^{d} \frac{1}{2d}\delta^\mu_\lambda \delta^\nu_\lambda$$

$$= \frac{1}{d}\delta^{\mu\nu} = \sigma_0^2 \delta^{\mu\nu},$$

as we saw in class.

b) Consider the body centered cubic lattice

$$BCC = \mathbb{Z}\vec{a}_1 \oplus \mathbb{Z}\vec{a}_2 \oplus \mathbb{Z}\vec{a}_3$$

with

$$\vec{a}_1 = \frac{a}{2}(-1,1,1),$$

$$\vec{a}_2 = \frac{a}{2}(1,-1,1),$$

$$\vec{a}_3 = \frac{a}{2}(1,1,-1).$$

We consider a random walk on BCC where at every step the probability is

$$P(\vec{v}) = \begin{cases} \frac{1}{8} & \vec{v} \in bcc := \pm\{\vec{a}_1, \vec{a}_2, \vec{a}_3, \vec{a}_1+\vec{a}_2+\vec{a}_3\} \\ 0 & \vec{v} \notin bcc. \end{cases}$$

Thus, the probability of being at $\vec{r} \in BCC$ after n steps is

$$P_n(\vec{r}) = \sum_{\vec{v} \in bcc} P_{n-1}(\vec{r}-\vec{v})P(\vec{v}), \qquad P_0(\vec{r}) = \delta_{\vec{r},\vec{0}}$$

Define

$$\tilde{P}_n(\vec{k}) = \sum_{\vec{r} \in BCC} e^{-i\vec{k}\cdot\vec{r}} P_n(\vec{r}).$$

Thus, we need to find a region Ω and N so that

$$P_n(\vec{r}) = N\int_{\Omega} d^3\vec{k}\, e^{i\vec{k}\cdot\vec{r}} \tilde{P}_n(\vec{k}) = N\sum_{\vec{r}' \in BCC} \int_{\Omega} d^3\vec{k}\, e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} P_n(\vec{r}'),$$

i.e.

$$\mathcal{N}\int_{\Omega} d^3\vec{k}\, e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')} = \delta_{\vec{r},\vec{r}\,'}, \quad \text{for all } \vec{r},\vec{r}\,' \in BCC$$

Let $\{\vec{b}^1,\vec{b}^2,\vec{b}^3\}$ be a basis of $\mathbb{R}^3$ s.t.

$$\vec{b}^i\cdot\vec{a}_j = \delta^i{}_j$$

Let Q be the change of coordinate matrix from the canonical basis to $\{\vec{b}^1,\vec{b}^2,\vec{b}^3\}$. Then, if $Q(\Omega) = [-\pi,\pi]^d$ and $\vec{r}-\vec{r}\,' = n^i\vec{a}_i \in BCC$ for $n^1,n^2,n^3 \in \mathbb{Z}$, we have

$$\mathcal{N}\int_{\Omega} d^3\vec{k}\, e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')} = \mathcal{N}\int_{[-\pi,\pi]^3} d^3\vec{q}\, \frac{1}{|\det Q|}\, e^{iq_i\vec{b}^i\cdot(\vec{r}-\vec{r}\,')} = \frac{(2\pi)^3\mathcal{N}}{|\det Q|}\,\delta_{\vec{n},\vec{0}}\,.$$

Then clearly $\mathcal{N} = \dfrac{|\det Q|}{(2\pi)^3}$ and

$$\Omega = [-\pi,\pi]\,\vec{b}^1 \oplus [-\pi,\pi]\,\vec{b}^2 \oplus [-\pi,\pi]\,\vec{b}^3.$$

Moreover, $\dfrac{1}{|\det Q|}$ is the volume of Ω, $|\det(\vec{b}^1,\vec{b}^2,\vec{b}^3)|$, or rather, $1/|\det Q|$ is the volume of the primitive cell

$$|\det(\vec{a}_1,\vec{a}_2,\vec{a}_3)| = \frac{a^3}{8}\begin{vmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix}$$

$$= \frac{a^3}{8}\Big(-1(1-1)-1(-1-1)+1(1+1)\Big)$$

$$= \frac{a^3}{2},$$

and

$$P_n(\vec{r}) = \frac{d^3}{2}\int_{\Omega'}\frac{d^3\vec{k}}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{r}}\,\hat{P}_n(\vec{k}).$$

The vectors $\vec{b}^1, \vec{b}^2, \vec{b}^3$ can be taken to be

$$\vec{b}^1 = \frac{\vec{a}_2\times\vec{a}_3}{d^3/2} = \frac{2}{d^3}\frac{d^2}{4}(0,2,2) = \frac{1}{d}(0,1,1)$$

$$\vec{b}^2 = \frac{\vec{a}_3\times\vec{a}_1}{d^3/2} = \frac{2}{d^3}\frac{d^2}{4}(-1+1,1-1,1+1) = \frac{1}{d}(1,0,1)$$

$$\vec{b}^3 = \frac{1}{d}(1,1,0).$$

In terms of these fourier transforms we have

$$\hat{P}_{n+1}(\vec{k}) = \sum_{\vec{r}\in BCC} e^{-i\vec{k}\cdot\vec{r}}P_{n+1}(\vec{r}) = \frac{1}{8}\sum_{\vec{v}\in bcc}\ \sum_{\vec{r}\in BCC} e^{-i\vec{k}\cdot\vec{r}}P_n(\vec{r}-\vec{v})$$

$$= \frac{1}{8} \sum_{\vec{v} \in bcc} \sum_{\vec{r} \in BCC} e^{-i\vec{K}\cdot(\vec{r}+\vec{v})} P_n(\vec{r})$$

$$= \frac{1}{8} \sum_{\vec{v} \in bcc} e^{-i\vec{K}\cdot\vec{v}} \tilde{P}_n(\vec{K}).$$

On the other hand

$$\tilde{P}_0(\vec{K}) = \sum_{\vec{r} \in BCC} e^{-i\vec{K}\cdot\vec{r}} \delta_{\vec{r},\vec{0}} = 1.$$

Thus

$$\tilde{P}_n(\vec{K}) = \left(\frac{1}{8} \sum_{\vec{v} \in bcc} e^{-i\vec{K}\cdot\vec{v}} \right)^n$$

and

$$P_n(\vec{r}) = \frac{d^3}{2} \int_{\Omega} \frac{d^3\vec{K}}{(2\pi)^3} e^{i\vec{K}\cdot\vec{r}} \left(\frac{1}{8} \sum_{\vec{v} \in bcc} e^{-i\vec{K}\cdot\vec{v}} \right)^n$$

$$= \frac{d^3}{2\cdot 8^n} \int_{\Omega} \frac{d^3\vec{K}}{(2\pi)^3} e^{i\vec{K}\cdot\vec{r}} \sum_{\vec{v}_1 \in bcc} e^{-i\vec{K}\cdot\vec{v}_1} \cdots \sum_{\vec{v}_n \in bcc} e^{-i\vec{K}\cdot\vec{v}_n}$$

$$= \frac{d^3}{2\cdot 8^n} \sum_{\vec{v}_1,\dots,\vec{v}_n \in bcc} \int_{\Omega} \frac{d^3\vec{K}}{(2\pi)^3} e^{i\vec{K}\cdot\left(\vec{r} - \sum_{i=1}^{n} \vec{v}_i\right)}.$$

Thus, if $\|\vec{r}\| > n\|\vec{a}_1\| = n\|\vec{a}_2\| = n\|\vec{a}_3\| = n\frac{a}{2}\sqrt{3} = \frac{\sqrt{3}a}{2} n$

we have that for all $\vec{v}_1,\dots,\vec{v}_n \in bcc$

$$\left\| \sum_{i=1}^{n} \vec{v}_i \right\| \leq \sum_{i=1}^{n} \| \vec{v}_i \| = \sum_{i=1}^{n} \frac{\sqrt{3}\,a}{2} = \frac{\sqrt{3}\,a}{2} n < \| \vec{r} \| .$$

In particular $\vec{r} \neq \sum_{i=1}^{n} \vec{v}_i$ and

$$P_n(\vec{r}) = \vec{0}.$$

c) Much like before, for big n and $\vec{r}$

$$P_n(\vec{r}) = \frac{a^3}{2} \int_{\Omega} \frac{d^3\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}} \left(\frac{1}{4} \left(\cos(\vec{k}\cdot\vec{a}_1) + \cos(\vec{k}\cdot\vec{a}_2) + \cos(\vec{k}\cdot\vec{a}_3) + \cos\left(\vec{k}\cdot(\vec{a}_1+\vec{a}_2+\vec{a}_3)\right)\right)\right)^n$$

$$= \frac{a^3}{2} \int_{\Omega} \frac{d^3\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}} \left(\frac{1}{4} \left(1 - \frac{1}{2}(\vec{k}\cdot\vec{a}_1)^2 + 1 - \frac{1}{2}(\vec{k}\cdot\vec{a}_2)^2 + 1 - \frac{1}{2}(\vec{k}\cdot\vec{a}_3)^2 + 1 - \frac{1}{2}(\vec{k}\cdot(\vec{a}_1+\vec{a}_2+\vec{a}_3))^2 + \mathcal{O}(\|\vec{k}\|^4) \right)\right)^n$$

$$= \frac{a^3}{2} \int_{\Omega} \frac{d^3\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}} \left(1 - \frac{1}{8}\left((\vec{k}\cdot\vec{a}_1)^2 + (\vec{k}\cdot\vec{a}_2)^2 + (\vec{k}\cdot\vec{a}_3)^2 + (\vec{k}\cdot(\vec{a}_1+\vec{a}_2+\vec{a}_3))^2\right) + \mathcal{O}(\|\vec{k}\|^4)\right)^n$$

As expected, we obtain no bias

$$(\vec{k}\cdot\vec{a}_1)^2 + (\vec{k}\cdot\vec{a}_2)^2 + (\vec{k}\cdot\vec{a}_3)^2 + (\vec{k}\cdot(\vec{a}_1+\vec{a}_2+\vec{a}_3))^2$$

$$= \frac{a^2}{4}\left[(-k_1+k_2+k_3)^2 + (k_1-k_2+k_3)^2 + (k_1+k_2-k_3)^2 + (k_1+k_2+k_3)^2 \right]$$

$$= \frac{a^2}{4}\left[4(k_1^2+k_2^2+k_3^2) + 2\left(-\cancel{k_1k_2} - \cancel{k_1k_3} + \cancel{k_2k_3} - \cancel{k_1k_2} + \cancel{k_1k_3} - \cancel{k_2k_3} + \cancel{k_1k_2} - \cancel{k_1k_3} - \cancel{k_2k_3} + \cancel{k_1k_2} + \cancel{k_1k_3} + \cancel{k_2k_3}\right)\right] = a^2\|\vec{k}\|^2.$$

We conclude

$$P_n(\vec{r}) = \frac{a^3}{2}\int_\Omega \frac{d^3\vec{k}}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{r} - \frac{nd^2}{8}\|\vec{k}\|^2} + \Theta(\|\vec{k}\|^4)$$

?

$$\therefore \approx \int \frac{d^3\vec{k}}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{r} - n\frac{d^2}{8}\|\vec{k}\|^2}$$

$$= \frac{1}{(2\pi)^3}\left(\frac{2\pi}{nd^2/4}\right)^{3/2} e^{-\vec{r}^2/nd^2/2}$$

$$= \frac{1}{n^{3/2}}\frac{1}{(2\pi\, d^2/4)^{3/2}}\, e^{-\vec{r}^2/2nd^2/4}$$

i.e. after rescaling, we flow to a gaussian with standard deviation $d/2$. Moreover, just like before, $\frac{d}{2}$ corresponds to the second moment of P. Indeed, noting that

$$a_i^\mu = \frac{d}{2}(1 - 2\delta_i^\mu),$$

$$a_3^\mu = \frac{a}{2},$$

we have

$$\langle x^\mu x^\nu\rangle = \frac{1}{8}\sum_{\vec{v}\in bcc} v^\mu v^\nu = \frac{1}{4}\frac{a^2}{4}\left(\sum_{i=1}^{3}(1 - 2\delta_i^\mu - 2\delta_i^\nu + 4\delta_i^\mu\delta_i^\nu) + 1\right)$$

$$= \frac{1}{4}\frac{a^2}{4}\left(\cancel{4} - \cancel{2} - \cancel{2} + 4\delta^{\mu\nu}\right) = \frac{a^2}{4}\delta^{\mu\nu}.$$

d) We have

$$G(1,\vec{a}) = \sum_{n=0}^{\infty} P_n(\vec{r})$$

$$= \frac{2}{a^3}\int_{BZ} \frac{d^3\vec{k}}{(2\pi)^3} \frac{1}{1 - \frac{1}{4}\left(\cos(\vec{k}\cdot\vec{a}_1) + \cos(\vec{k}\cdot\vec{a}_2) + \cos(\vec{k}\cdot\vec{a}_3) + \cos(\vec{k}\cdot(\vec{a}_1 + \vec{a}_2 + \vec{a}_3))\right)}$$

$$= \int_{[-\pi,\pi]^3} \frac{d^3\vec{q}}{(2\pi)^3} \frac{1}{1 - \frac{1}{4}\left(\cos(q_1) + \cos(q_2) + \cos(q_3) + \cos(q_1 + q_2 + q_3)\right)}$$

$$\approx 1.39301.$$

After Alexandre gave me a tip to avoid all of this Fourier theory, we find the following solution.

We have

$$P_n(\vec{r}) = \sum_{\vec{v}_1,\dots,\vec{v}_n \in bcc} \delta_{\vec{r},\sum_{i=1}^{n}\vec{v}_i} \frac{1}{8^n}$$

$$= \sum_{\vec{v}_1,\dots,\vec{v}_n \in bcc} \frac{1}{8^n} \int_{[-\pi,\pi]^3} \frac{d^3\vec{q}}{(2\pi)^3} e^{i\vec{q}\cdot\left(\vec{r}-\sum_{i=1}^{n}\vec{v}_i\right)} .$$

At this point we can argue like before to show that the random walker must be a finite distance away from the origin. To compute the long distance behaviour we have

$$P_n(\vec{r}) = \int_{[-\pi,\pi]^3} \frac{d^3\vec{q}}{(2\pi)^3} e^{i\vec{q}\cdot\vec{r}} \left(\frac{1}{8}\sum_{\vec{v}\in bcc} e^{-i\vec{q}\cdot\vec{v}}\right)^n .$$

In here we recover our integral in part c). However, there is no extra factor of $\frac{d^3}{2}$ and the integration region is the correct one. We thus get the long distance limit we obtained before without the sketchy step

$$\frac{d^3}{2}\int_{\Omega} \longrightarrow \int_{\mathbb{R}^3}$$

and instead the more reasonable

$$\int_{[-\pi,\pi]^3} d^3\vec{q} \to \int_{\mathbb{R}} d^3\vec{q}.$$

Thus

$$P_n(\vec{r}) = \frac{1}{n^{3/2}} \frac{1}{(2\pi a^2/4)^{3/2}} e^{-\vec{r}^2/2\pi a^2/4}.$$

However our solution to problem d) does change because we instead have

$$G(1,\vec{0}) = \int_{[-\pi,\pi]^3} \frac{d^3\vec{q}}{(2\pi)^3} \frac{1}{1-\frac{1}{4}\left(\sum_{i=1}^{3}\cos(\vec{q}\cdot\vec{a}_i) + \cos\left(\vec{q}\cdot\sum_{i=1}^{3}\vec{a}_i\right)\right)}$$

$$= 1. \qquad a = 2$$

~~These results, although seemingly transparent, have the undesired feature that the last question depends on a. This is undesired since P is a independent Moreover, both of the values calculated are bigger than the hypercubic value. This doesn't make sense since the bcc has more neighbors than the hypercubic and, thus, should diffuse faster.~~

This result agrees with our intuition that if we have more nearest neighbours then difussion is easier. Comparing with Whon Zehn, this is the correct intuition. Indeed, for the fcc she obtained $\sim 1.39\ldots$ and this lattice has 12 nearest neighbours.

e) Microscopic details affect the actual numeric result of $G(1,\vec{r})$. However, im the 3 cases studied we arrived to the same form

$$G(1,\vec{r}) = \int_{[-\pi,\pi)^3} \frac{d^3\vec{q}}{(2\pi)^3} \frac{e^{i\vec{q}\cdot\vec{r}}}{1 - \#\text{ nearest neighors } F(\vec{q})}$$

for a highly symmetric $f(\vec{q})$.