Multipolar diffusion

Ethan Lake

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Generalities

First let us understand what types of "diffusive" behavior we expect to find in lattice gases whose dynamics is multipole moment conserving. The setting we have in mind is a lattice gas where particles hop in a multipole-conserving way, with the probability of a given hopping event occurring being proportional to the total number of distinct groups of particles¹ that can be selected to hop. For example with only charge (0-pole) conservation, a hopping process which moves a particle on site i to a site $j \neq i$ will have a probability of occurring proportional simply to the number of particles on site i, ρ_i . A dipole-conserving hopping process which moves a pair of particles at sites (i, j) to sites $(i + \delta, j - \delta)$ has an occurance probability proportional to the number of pairs that can be selected to hop, viz.

$$P_{(i,j)\to(i+\delta,j-\delta)} \propto \rho_i \rho_j.$$
 (1)

Higher multipole moments are similar.

The above rule for the hopping probabilities amounts to taking a "mean-field" limit, with the probability for a multipole-conserving hop factorizing in terms of a product of the densities ρ_i at the sites where the hopping occurs. While this factorization is not generic per se, note that any possible hopping probability must vanish if any of the ρ_i do, thus e.g. the dipole hopping probability $P_{(i,j)\to(i+\delta,j-\delta)}$ must vanish when either ρ_i or ρ_j do. The product form above is the simplest rule compatible with this constraint.

For simplicity we will mostly restrict ourselves to the multipole group of degree n in 1d, with the dynamics conserving

$$Q^{(m)} \equiv \int_x x^m \rho_x \qquad \forall \ m \le n. \tag{2}$$

¹viewing the particles as being distinguishable.

Note that translation invariance plus conservation of $Q^{(n)}$ automatically imply conservation of all $Q^{(m)}$ for $m \leq n$. In this case, while the value of $Q^{(m)}$ is only independent of the choice of origin if $Q^{(o < m)} = 0$ for all o, the conservation of $Q^{(m)}$ is true independently of the choice of origin.

Generalizing to higher dimensions can be done easily if we generalize to the maximal multipole group, i.e. if the dynamics conserves $\int_{\mathbf{r}} p_n(r_a) \rho_{\mathbf{r}}$ for all degree-n polynomials of the coordinates r_a . Non-maximal multipole groups (where e.g. one has a conservation law for $p_n(r_a) = x^2, y^2$ but not xy) are more complicated and will only be briefly touched on.

Translation invariance and conservation of the n-pole moment requires the continuity equation to look like

$$\partial_t \rho = \partial_{I_n} J^{I_n},\tag{3}$$

where $I_n = \{i_1, \dots, i_n\}$ is a composite index. The most natural thing to write—and indeed what most people in the literature seem to do—is to take

$$J^{I_n} \stackrel{?!}{=} D\partial^{I_n} \rho. \tag{4}$$

This however gives a linear (sub) diffusion equation, which cannot be right in our model, since the kinetic constraints force the dynamics to freeze out when $\rho \to 0$. Another way of saying this is that since the probabilities for a given hopping event are nonlinear in ρ (as long as n > 0), the constitutive relation for the current must also be nonlinear in ρ . One guess of how to fix this would be to let D simply be proportional to ρ raised to an appropriate power, capturing the fact that diffusion becomes frozen out at low densities. Luckily, this (rather boring) solution also turns out to be incorrect.

equilibrium

A slightly hacky² way of seeing this is to find the steady states of the density that arise when we maximize the entropy—which in the current context is just $S = -\int_x \rho_x \ln \rho_x$ —subject to the constraints of having fixed multipole moments. Doing this gives

$$\rho_x^{eq} = \exp\left(\sum_{m=0}^n \lambda_m x^m\right),\tag{5}$$

where the Lagrange multipliers λ_m are determined from the values of the multipolar charges by $\int_x x^m \rho_x = Q^{(m)}$. The fact that we get exponential functions as steady-state solutions to our multipolar diffusion processes guarantees that we cannot simply take the multipolar current J to be linear in ρ , as we need J to vanish on solutions of the form (5).

²I describe this argument as being "hacky" since it relies on entropy maximization, while the systems we are considering are not ergodic for any strictly local implementation of dipole-conserving dynamics. Complaining about ergodicity is rather legalistic though, as we will always be interested in the dynamics that occurs in sectors that occupy "very big" subsets of configuration space, and here the dynamics will be ergodic enough that the microcanonical and grand canonical approaches will agree.

For illustration consider the n=1 case of dipole conservation, and let the system live in a box with $x \in [-L/2, L/2]$. Then the equilibrium distribution is

$$\rho_{\rm eq}(x) = e^{-\beta(x-\mu)}, \qquad \mu = \frac{1}{\beta} \ln \left(\frac{N}{2\beta \sinh(L/2\beta)} \right), \tag{6}$$

where β solves the equation

$$x_{\rm cm} \equiv \frac{Q^{(1)}}{L} = \frac{1}{\beta} - \frac{L}{2} \coth(L\beta/2). \tag{7}$$

Note that we are at "infinite temperature" $\beta = 0$ (giving a uniform density distribution) when $x_{\rm cm} = 0$ (or if $L \to \infty$ and $x_{\rm cm}$ is finite); in all other cases we obtain an exponentially concetrated steady-state profile which hugs one of the edges of the box. In particular, when $x_{\rm cm} = -L/2$ we obtain a $T = 0^+$ "zero temperature" state with all of the particles on the left boundary, while when $x_{\rm cm} = L/2$ we obtain a $T = 0^-$ "barely negative temperature" state with all of the particles on the right boundary.

When we think from the perspective of the dynamics, the fact that the particles end up localizing themselves despite the "infinite temperature" (rejection-free) nature of the dynamics may seem surprising, but in the interpretation above it is not surprising at all: as far as the equilibrium state is concerned, we are simply studying the statistical physics of particles in a linear potential, with the steady-state of course being one in which the particles are clumped at one end of the system or another.

minimal nonlinearities of the consitutive relation

To determine the kinds of multipolar diffusion equations that have (5) as solutions, we start by lower-bounding the number of powers of ρ that must enter into the constitutive relation. To this end, in this subsection we prove the following proposition:

Proposition 1. For dynamics that conserves the n-pole moment of the charge, the constitutive relation expressing the current in terms of the density must involve at least n+1 powers of ρ and n+1 spatial derivatives. This lower bound can be saturated for at least all $n \leq 10$.

f>. Let us first determine the minimal number of powers of ρ that must appear
in the constitutive relation for the current. This number is determined by finding
the smallest number of particles that can participate in an n-pole preserving particle
hopping process. For a process involving m particles, let $\mathbf{a}, \mathbf{b} \in \mathbb{Z}^m$ denote the initial
and final positions of the particles, respectively. Note that if $a_i = b_j$ for any $i, j \in$ $1, \ldots, m$, then at least one particle does not actually move during the hopping process;
thus wolog we may restrict to $\{a_i\} \cap \{b_i\} = \emptyset$. If the process $\mathbf{a} \mapsto \mathbf{b}$ is to preserve all
multipole moments up to n, we require that

$$\sum_{i} a_i^p = \sum_{i} b_i^p \ \forall \ p \in \{0, \dots, n\}.$$

$$(8)$$

The goal is thus to find the smallest-length pair of disjoint integer-valued sets such that the above equation is satisfied.

We now show that (8) can be satisfied only when m > n. Indeed, suppose that m = n. It is a well-known fact [2] that the set of "power-sum polynomials"

$$P_q(\mathbf{a}) \equiv \sum_{i=1}^m a_i^q \tag{9}$$

for $q \in \{0, ..., m\}$ generate all symmetric polynomials in m variables (not over \mathbb{Z} , but over \mathbb{Q} , although this doesn't matter for us). This means that the symmetric polynomials $\prod_{i=1}^m a_i, \prod_{i=1}^m b_i$ can be expressed as \mathbb{Q} -valued linear combinations of the $P_q(\mathbf{a}), P_q(\mathbf{b})$, respectively. But since we have assumed that all $o \leq m$ multipole moments are conserved, we have

$$P_q(\mathbf{a}) = P_q(\mathbf{b}) \ \forall \ q \in \{0, \dots, m\} \implies \prod_{i=1}^m a_i = \prod_{i=1}^m b_i. \tag{10}$$

Now we use the fact that (8) is invariant under translations, in that (8) implies

$$P_q(\mathbf{a} - x) = P_q(\mathbf{b} - x) \tag{11}$$

for any constant vector x (this follows from the fact that $P_q(\mathbf{a}-x)$ is also a symmetric polynomial). In particular, we may choose $x=a_1$ to effectively set $a_1=0$ wolog. But then from the above we see that since $\prod_i a_i=0$, we must also have $\prod_i b_i=0$. In particular, one of the b_i must equal zero, which contradicts our assumption about the disjointness of $\{a_i\}, \{b_i\}$.

This shows that any n-pole conserving hopping process must involve at least n+1 particles, so that the constitutive relation must involve at least n+1 powers of the density. This also implies that the current must involve at least n+1 derivatives; if it involved fewer than n+1 derivatives then it would be proportional to an overall power of the density $J = \rho^k(\cdots)$ (where \cdots involves derivatives of ρ), and the ρ^k in front could be stripped away without affecting the nature of the zero-current solutions.

</proof>

We have shown that n+1-body terms are necessary, but not that they are sufficient. Showing this would amount to proving that one can always find two mutually disjoint size-n+1 sets of integers satisfying (8). Such solutions are known to exist for $n \leq 10$ and n = 12, but for other values of n the answer is unknown, and the full resolution of this question is in fact a famous open problem in number theory [1] known as the Prouhet-Tarry-Escott problem.

The explicit solutions of (8) quickly get rather complicated for large n, meaning that they involve very long-range hopping processes. For example, when n = 7 the simplest solution has an eight-body hopping process with

$$a = [1, 5, 10, 24, 28, 42, 47, 51]$$

$$b = [2, 3, 12, 21, 31, 40, 49, 50]$$
(12)

meaning that the minimal-body hopping process extends over 50 lattice sites.

Depending on the physical context it may be unreasonable to consider such longrange hopping terms, instead considering shorter-range but higher-body hopping processes. The minimal-range hopping processes involve a number of particles that scales exponentially in n but has range equal to n + 2, which can be constructed by letting

$$\mathbf{a} = \bigoplus_{i=0}^{\lfloor (n+1)/2 \rfloor} (2i)^{\oplus \binom{n+1}{2i}}, \qquad \mathbf{b} = \bigoplus_{i=1}^{\lfloor (n+2)/2 \rfloor} (2i-1)^{\oplus \binom{n+1}{2i-1}}, \tag{13}$$

where \oplus denotes concatenation, so that e.g. $x^{\oplus k}$ is the length-k vector with all entries equal to x. For dipoles this gives the 2-body process $\mathbf{a} = (1,3)$, $\mathbf{b} = (2,2)$, for quadrupoles the 4-body process $\mathbf{a} = (1,3,3,3)$, $\mathbf{b} = (2,2,2,4)$, and so on.

scaling

Consider a value of n for which the minimal number of powers of ρ appearing in the expression for the current is the minimum value of n+1 (as we saw above this will always be satisfied for all "reasonable" choices of n). Since the current will then contain n+1 powers of ρ and n+1 spatial derivatives, a single-variable scaling ansatz $\rho(x,t) = \rho(xt^{-1/z})$ yields

$$z = n(2+d) + 2. (14)$$

This is quite striking in that it explicitly depends on d, which is not something that happens for the regular (linear) diffusion equation (n = 0).

However, this single-variable scaling ansatz actually is only applicable in the cases of n = 0, 1. Indeed, suppose that n > 1. Then both $Q^{(0)}$ and $Q^{(2)}$ must be time-independent, which is impossible if $\rho(x,t) = \rho(xt^{-1/z})$, except in the trivial case when $Q^{(0)} = Q^{(2)} = 0$ or if we ignore (14) and take $z = \infty$. Physically, when n > 1 we always have a non-zero conserved quadrupole moment that defines a length scale in the problem.

For dipolar diffusion, a single-variable scaling ansatz works because we can always choose to define $Q^{(1)}$ with the origin located at $x_{\rm cm}$, so that $Q^{(1)}=0$. Thus when $Q^{(1)}$ is conserved but $Q^{(2)}$ is not, we expect that $Q^{(2)}$ evolves over time as

$$Q^{(2)}(t) \sim t^{\frac{1}{4+d}}. (15)$$

Master equation and scaling limit

In this section we will derive the multipolar diffusion equations from lattice master equations. Doing so will require us to think about how to take a scaling limit where derivative expansions become valid, which conceptually works out in a way rather different as compared to conventional diffusion.

conventional diffusion

We begin by reviewing conventional diffusion. Let n_i be the number of particles on site i. If the probability for a single particle to hop within a time step dt is r, then

$$\partial_t n_i = \frac{r}{dt} (n_{i+1} + n_{i-1} - 2n_i). \tag{16}$$

Let a be the lattice spacing and $\mathcal{N} \in \mathbb{N}$ be the number of sites. Define the density $\rho_x \equiv n_i/a$, where the switch between i and x is merely suggestive notation. Consider the continuum limit, where $a \to 0$ with fixed $\mathcal{N}a$; here we usually say that we may take $x \in \mathbb{R}$ and that ρ_x is well-defined in this limit, meaning that ρ_x is some O(1) number at any given $x \in \mathbb{R}$. In terms of the original lattice model, this means that the average occupancy of any lattice site is $n_i \sim a\rho_x \to 0$. This makes sense for thinking about the continuum — we hold fixed the total number of particles but increase the number of lattice spacings between particles, while at the same time making the lattice spacing smaller. In the continuum limit we would not usually take n_i to be O(1), since then ρ_x does not have a well-defined limit. For the diffusion equation this is okay because it is non-interacting, and the way in which a large number of particles diffuse is asymptotically equal to the average way that a single particle diffuses. Thus having the lattice limit be dilute is acceptable.

In the continuum limit we write the lattice diffusion equation as

$$\partial_t \rho_x = D \left(\partial_x^2 \rho_x + \frac{a^2}{12} \partial_x^4 \rho_x + \cdots \right), \qquad D \equiv \frac{ra^2}{dt}.$$
 (17)

We then drop the higher order derivative terms on the grounds that $a \to 0$ and that all derivatives $\partial_x^n \rho$ are of the same size.

dipolar diffusion

Now we move on the to dipolar case. Consider a master equation generated by the processes $0110 \leftrightarrow 1001$. Then

$$\partial_t n_i = \frac{r}{dt} \left(n_{i-1} n_{i+2} + n_{i-2} n_{i+1} + n_{i+1} n_{i+2} + n_{i-1} n_{i-2} - n_i (n_{i+1} + n_{i-1} + n_{i+3} + n_{i-3}) \right). \tag{18}$$

Again define $\rho = n/a$. Then

$$\partial_t \rho_x = \frac{4ra^5}{dt} \partial_x^2 \left((\partial_x \rho)^2 - \rho \partial_x^2 \rho + a^2 (\cdots) \right), \tag{19}$$

where the \cdots have two ρ s and six ∂ s. Dropping the (\cdots) , the zero-current solutions are exponentials:

$$\rho^{\text{eq}}(x) = e^{\lambda x}. (20)$$

It is illuminating to also consider the master equation generated by $020 \leftrightarrow 101$. Since the number of pairs to be chosen when two particles hop from the same site is $n_i(n_i-1)$ — instead of n_i^2 — we get

$$\partial_t n_i = \frac{r}{dt} \left(2n_{i-1}n_{i+1} + n_{i+1}(n_{i+1} - 1) + n_{i-1}(n_{i-1} - 1) - n_i(2(n_i - 1) + n_{i+2} + n_{i-2}) \right). \tag{21}$$

This becomes

$$\partial_t \rho_x = \frac{ra^5}{dt} \partial^2 ([(\partial_x \rho)^2 - \rho \partial_x^2 \rho + a^2(\cdots)] - a^{-3}\rho). \tag{22}$$

Note in particular the appearance of the $-\frac{ra^2}{dt}\partial_x^2\rho$ term on the RHS, which acts as a conventional diffusion term with *negative* diffusion constant, thereby favoring charge

localization (as before the \cdots represents terms with two ρ s and six ∂_x s). Dropping the (\cdots) , the zero-current solutions are now

From (19) one might be tempted to take a continuum limit by letting $D = 4ra^5/dt$ be a constant (the power of a^5 is weird but we can scale dt with whatever z we wish) and taking $\rho, \partial \rho, \dots \sim O(1)$. But in this limit the 3-site master equation is not well defined, possessing an infinitely negative diffusion term which completely localizes all of the particles. In fact this localization is very physical: in the continuum limit the particles in the lattice regularization are very dilute, and we know that in the dilute limit dipole-conserving particles are completely frozen, with trivial dynamics.

Thus interesting (non-frozen) dynamics does not occur in the continuum limit.

quadrupolar diffusion

A master equation containing only cubic terms in the n_i can be obtained by considering the process

$$1000110 \leftrightarrow 0110001.$$
 (24)

A simpler (but still 3-body) process is $20010 \leftrightarrow 01002$. Because of the 2s, this process will contain a contribution to the current which is only quadratic in n_i . Indeed, the full master equation is

$$\frac{dt}{r}\partial_t n_i = 2n_{i-2}(n_{i-2}-1)n_{i+1} + n_{i+1}(n_{i+1}-1)n_{i+4} + 2n_{i-1}n_{i+2}(n_{i+2}-1) + n_{i-4}n_{i-1}(n_{i-1}-1) - n_i\left(2(n_i-1)n_{i+3} + n_{i-3}(n_{i-3}-1) + n_{i+3}(n_{i+3}-1) + 2(n_i-1)n_{i-3}\right).$$
(25)

Expanding in derivatives,

$$\partial_t \rho_x = \frac{2ra^8}{dt} \partial_x^3 \left(\left[\rho^3 \partial_x^3 \ln(\rho) + a^2(\cdots) \right] + a^{-3} \rho \partial_x \rho \right). \tag{26}$$

Examples

dipole

Consider first dipolar diffusion in 1d. We know the current will have n+1=2 powers of ρ and also n+1=2 derivatives. Thus

$$J = a(\partial_x \rho)^2 + b\rho \partial_x^2 \rho \tag{27}$$

for some a, b, determined by requiring that J = 0 when evaluated on any entropy-maximizing function of the form $\rho(x) = e^{\lambda x}$. It is easy to check that a = 1, b = -1 is required, thus yielding the dipolar diffusion equation

$$\partial_t \rho = D \partial_x^2 ((\partial_x \rho)^2 - \rho \partial_x^2 \rho). \tag{28}$$

An interesting fact is that this equation (along with the higher multipole version to follow) is not conservative, meaning that the RHS cannot be written as $\delta H(\rho)/\delta \rho$

for any function $H(\rho)$. To see this, note that any such $H(\rho)$ must involve three powers of ρ and four derivatives. We can thus generally write such an H as

$$H = a\partial^4 \rho \rho^2 + b\rho \partial^3 \rho \partial \rho + c\rho (\partial^2 \rho)^2 + d\rho (\partial \rho)^2 \partial^2 \rho. \tag{29}$$

To see this, we write the RHS as $D[(\partial \rho)^2 - \rho \partial^4 \rho]$.

quadrupole

Consider now quadrupolar conservation, and remain in 1d. We know the current needs to have n+1=3 powers of ρ , as well as 3 derivatives. Thus the minimal expression for the current reads

$$J = a\rho^2 \partial_x^3 \rho + b\rho \partial_x \rho \partial_x^2 \rho + c(\partial_x \rho)^3, \tag{30}$$

where a, b, c are to be determined by requiring that J = 0 when evaluated on any entropy-maximizing function of the form $\rho(x) \propto e^{-(x-x_0)^2/2\sigma^2}$. A bit of algebra shows that the correct choice is to let a = -1, b = 3, c = -2. Thus the minimal quadrupolar diffusion equation is

$$\partial_t \rho = D\partial_x^3 \left(-2(\partial_x \rho)^3 - \rho^2 \partial_x^3 \rho + 3\rho \partial_x \rho \partial_x^2 \rho \right). \tag{31}$$

The above equation is indeed what is derived when one performs a graident expansion on the quadrupole-conserving 3-body process (-1, 2, 0, -2, 1), viz. $\mathbf{a} = (1, 4, 4)$, $\mathbf{b} = (2, 2, 5)$. This can be easily verified by performing a gradient expansion on the microscopic current

$$J_i = \rho_{i-2}\rho_{i+1}^2 - \rho_{i-1}^2\rho_{i+2} \tag{32}$$

for which one obtains D=2 in the present units.

When one employs the shorter-ranged 4-body term $\mathbf{a} = (1, 3, 3, 3), \mathbf{b} = (2, 2, 2, 4),$ one instead obtains

$$\partial_t \rho = D \partial_x^3 \left(\rho [2(\partial_x \rho)^3 + \rho^2 \partial_x^3 \rho - 3\rho \partial_x \rho \partial_x^2 \rho] \right), \tag{33}$$

now with D=1, and with the extra power of ρ in the expression for the current. This is checked by performing a gradient expansion on the microscopic current, which for this hopping process reads

$$J_i = \rho_i^3 \rho_{i-2} - \rho_{i+1} \rho_{i-1}^3. \tag{34}$$

Thus the form of the derivatives in the constitutive relation is universal, but extra powers of ρ may always be tacked on by considering hopping processes with larger-than-necessary number of particles.

In infinite space, the asymptotic steady state is

$$\rho(x) = \frac{N}{\sqrt{2\pi Q^{(2)}}} e^{-(x - x_{\rm cm})^2 / 2Q^{(2)}}.$$
(35)

Thus we have the rather remarkable result that the system spontaneously "congeals" itself into a Gaussian blob, which then simply sits motionless motionelss for eternity. In a finite box one still gets a Gaussian solution, but the peak is no longer generically centered on $x_{\rm cm}$.

sextupole

The lowest-body sextupole-conserving process is a four-body process with $\mathbf{a} = (1, 4, 5, 8)$, $\mathbf{b} = (2, 2, 7, 7)$, while the shortest-range processes is an eight-body process obtained from Pascal's triangle as $\mathbf{a} = (1, 3, 3, 3, 3, 3, 3, 3, 5)$ $\mathbf{b} = (2, 2, 2, 2, 4, 4, 4, 4)$.

Since the minimal expression for the current should contain 4 powers of ρ and 4 derivatives, we may write

$$J = a(\partial \rho)^4 + b\rho^2 \partial \rho \partial^3 \rho + c\rho^2 \partial^2 \rho \partial^2 \rho + d\rho \partial^2 \rho (\partial \rho)^2 + e\rho^3 \partial^4 \rho$$
 (36)

for some constants a, b, c, d, e. Consider a solution of the form $\rho(x) = e^{f(x)}$. Then

$$J(x)e^{-f(x)} = f'^{4}(a+b+c+d+e) + f'^{2}f''(3b+2c+d+6e) + f''^{2}(c+3e) + f'f'''(b+4e).$$
(37)

Requring that $f(x) = \alpha x^3/3 + \beta(x-x_0)^2$ give a zero-current steady state solution for all α, β, x_0 is easily seen to be equivalent to the vanishing of the coefficients in each of the various derivative terms above. Solving this system equations then gives the sextupolar constitutive relation

$$J = D \left(6(\partial \rho)^4 + 4\rho^2 \partial \rho \partial^3 \rho + 3\rho^2 \partial^2 \rho \partial^2 \rho - 12\rho \partial^2 \rho (\partial \rho)^2 - \rho^3 \partial^4 \rho \right). \tag{38}$$

The correctness of this bad boy can be verified in the usual way by taking a gradient expansion of the microscopic current operator, which for the four-body process written above is

$$J_i = \rho_{i-2}^2 \rho_{i+3}^2 - \rho_{i-3} \rho_i \rho_{i+1} \rho_{i+4}, \tag{39}$$

which when expanded gives the above relation with D=6.

n-pole

By looking at the previous examples, we notice that they all conform to the pattern of

$$J = D\rho^{n+1}\partial^{n+1}\ln(\rho),\tag{40}$$

which certainly makes sense on account of the fact that $\rho(x)$ being an exponential of a degree n polynomial always yields a steady state. Nevertheless, the fact that the lower bound of n+1 on the number of particles that participate in an n-pole conserving hopping process is not tight means that the equation written above might not hold for very large values of n (e.g. n > 12).

subsystem symmetries

The situation in higher dimensions is similar if we restrict our attention to maximal multipole groups: in this case a J with n+1 derivatives in 1d is replaced by an n+1 component vector $J^{a_1...a_{n+1}}$, with each derivative getting its own index. While we will not investigate non-maximal multipole groups in much detail, one extreme example of interest is the subsystem symmetric case, where $\int_{\mathbf{r}} r_a^n \rho_{\mathbf{r}}$ is conserved for all n, but $\int_{\mathbf{r}} r_a^n r_b^m \rho_{\mathbf{r}}$ is not conserved as long as n, m > 0. As an example, in 2d the minimal hopping process consistent with this symmetry group (at least on the square lattice) is

the ring exchange term; it is easy to check that this produces the subsystem-symmetric diffusion equation

$$\partial_t \rho = D \partial_x \partial_y (\partial_x \rho \partial_y \rho - \rho \partial_x \partial_y \rho), \tag{41}$$

for which $\rho(\mathbf{r}) = e^{f(x)+g(y)}$ is a solution for any functions f, g. In keeping with this, any density configuration independent of either x or y is a steady state of the dynamics.

Adding noise

We now discuss a general framework for properly incorporating noise into the multipolar diffusion equations derived above. We will do this by making use of the generating functional approach, which allows us to derive (more general versions of) FDTs that set the standard deviation of the noise fields in terms of the diffusion constants. In the following we will consider multipole diffusion within the framework of a discrete-time Markov process with hopping rate r. We will also define the "jump" field $\hat{\Delta}_i(t) \equiv \hat{\rho}_i(t+\varepsilon) - \hat{\rho}_i(t)$, where the hats denote fields appearing in a spacetime path integral — expectation values of such fields will be denoted simply by dropping the hats. We also define the generating functional

$$W[\hat{\Gamma}] \equiv \langle e^{f \hat{\Gamma} \hat{\Delta}} \rangle, \tag{42}$$

where the expectation value is over all spacetime trajectories of $\hat{\rho}_i(t)$ (weighted by the probability for each configuration to occur), and $\Sigma \hat{\Gamma} \hat{\Delta}$ is shorthand for $\sum_t \sum_i \hat{\Gamma}_i(t) \hat{\Delta}_i(t)$. Functional derivatives of $\log W$ wrt $\hat{\Gamma}_i(t)$ can be used to generate connected correlation functions of the spacetime field $\partial_t \hat{\rho}_i$.

0-pole moment: standard diffusion

Let us first review how regular diffusion works. At a given timestep, $\hat{\Delta}_i(t)$ has a probability $zr\rho_i(t)$ of being -1 (here z is the coordination number of the lattice) and a $r\sum_{j\in\partial i}\rho_j(t)$ probability of being +1 (recall $\rho_i(t)=\langle \hat{\rho}_i(t)\rangle$). Thus in the $r\to 0$ continuum time limit, we obtain

$$W[\hat{\Gamma}] \approx \prod_{i,t} \left(1 + \frac{1}{2} r \sum_{j \in \partial i} (\rho_j(t) [e^{\hat{\Gamma}_i(t) - \hat{\Gamma}_j(t)} - 1] + \rho_i(t) [e^{-\hat{\Gamma}_i(t) + \hat{\Gamma}_j(t)} - 1] \right)$$

$$\rightarrow \exp \left(r \sum_{i,t} \sum_{j \in \partial i} \rho_j(t) (e^{\hat{\Gamma}_i(t) - \hat{\Gamma}_j(t)} - 1) \right), \tag{43}$$

where the -1s come from the possibility of no hopping events involving site i occuring, and the 1/2 on the first line comes from double-couting each hopping process. Differentiating with respect to $\hat{\Gamma}$, we get

$$\frac{\delta \ln W[\hat{\Gamma}]}{\delta \hat{\Gamma}_j(t)} = r \sum_{k \in \partial j} \left(\rho_k(t) e^{\hat{\Gamma}_j(t) - \hat{\Gamma}_k(t)} - \rho_j(t) e^{\Gamma_k(t) - \Gamma_j(t)} \right). \tag{44}$$

Sending $\hat{\Gamma}_i(t) \to 0$, we then see that

$$\partial_t \rho_i = r \sum_{j \in \partial_i} (\rho_j(t) - \rho_i(t)) \to D\partial_i^2 \rho_i(t),$$
 (45)

correctly reproducing the diffusion equation (letting $D \equiv ra^2$ with a the lattice spacing).

The power of the generating functional approach is that it lets us understand how to generalize the diffusion equation to a Langenvin equation in a way that properly accounts for the effects of noise. To see this, consider the second moment obtained by taking a functional derivative of (41):

$$\langle \partial_t \hat{\rho}_i \partial_{t'} \hat{\rho}_j \rangle_c = r \delta_{t,t'} \sum_{k \in \partial i} (\rho_j(t) + \rho_k(t)) (\delta_{ij} - \delta_{ik}). \tag{46}$$

Note that this expression passes the sanity checks of vanishing when we sum over either i or j, as it must due to $\partial_t Q^{(0)} = 0$:

$$\sum_{i} \langle \partial_t \hat{\rho}_i \partial_{t'} \hat{\rho}_j \rangle_c = \sum_{j} \langle \partial_t \hat{\rho}_i \partial_{t'} \hat{\rho}_j \rangle_c = 0. \tag{47}$$

Therefore we know that $\langle \partial_t \hat{\rho}_i \partial_{t'} \hat{\rho}_j \rangle_c = \delta_{t,t'} \partial_i \partial_j \mathcal{O}$ for some operator \mathcal{O} (here $\partial_i = \frac{\partial}{\partial x_i}$ and we are using notation appropriate for 1d, n.b~i is a lattice site and not the label of a spatial direction—sorry). Taking the continuum limit and expanding in derivatives gives³

$$\langle \partial_t \hat{\rho}_i \partial_{t'} \hat{\rho}_j \rangle_c = \delta_{t,t'} D \partial_i \partial_j ([\rho_i + \rho_j] \delta_{ij}). \tag{49}$$

Therefore we may write the Langevin equation as

$$\partial_t \hat{\rho}_i = D \partial_i^2 \rho_i(t) + \partial_i \eta(t), \tag{50}$$

where the noise field η_i has autocorrelators

$$\langle \eta_i(t)\eta_i(t')\rangle_c = 2D\delta_{t,t'}\delta_{ij}\rho_i(t). \tag{51}$$

Thus we have essentially derived a FDT, since the fluctuations of the noise are seen to be determined by the diffusion constant and the average density. The fact that it is the derivative of the noise field that appears on the RHS of the Langevin equation (rather than the noise field itself) is of course due to charge conservation.

It is rather unsavory that the standard deviation of the noise is explicitly dependent on the density, although physically this makes sense as absolute particle number fluctuations will be higher in regions with higher density. One might try to get around this by writing the noise term in the Langevin equation as $\partial_i(\sqrt{2D\rho_i}\widetilde{\eta}(t))$

$$\langle \partial_t \hat{\rho}_{\mathbf{r}} \partial_{t'} \hat{\rho}_{\mathbf{r}'} \rangle_c = \delta_{t,t'} D \sum_{a=1}^d \frac{\partial}{\partial r^a} \frac{\partial}{\partial r'^a} ([\rho_i + \rho_j] \delta_{ij}). \tag{48}$$

³In higher dimensions, this equation is written in more canonical notation as

where $\langle \widetilde{\eta}_i(t) \widetilde{\eta}_j(t') \rangle_c = \delta_{t,t'} \delta_{i,j}$, but this only works if one then writes $\partial_i \partial_j (\sqrt{\rho_i \rho_j} \delta_{ij}) \stackrel{?!}{=} \partial_i \partial_j (\rho_i \delta_{ij})$.

An application of this Langevin equation is the calculation of the structure factor that governs the spectrum of fluctuations about the equilibrium steady state. Write $\rho(x,t) = \rho^{eq}(x) + \gamma(x,t)$, where $\rho^{eq}(x)$ is a steady-state. Then in Fourier space, the Langevin equation is

$$\gamma = \frac{ik}{i\omega + Dk^2}\eta. \tag{52}$$

Now

$$\langle \eta_{k\omega} \eta_{q\nu} \rangle_c = 2D\delta_{\omega,-\nu} \rho_{k+q}^{\text{eq}}.$$
 (53)

We will assume that $\rho^{\text{eq}}(x)$ varies on scales much longer than the relevant fluctuations in η , so that ρ_{k+q}^{eq} can be approximated locally as $\rho^{\text{eq}}(x)\delta_{k,-q}$. Then the local correlation functions of γ read

$$\langle \gamma_{k\omega} \gamma_{k\omega}^* \rangle_c = 2D\rho^{\text{eq}}(x) \frac{k^2}{\omega^2 + D^2 k^4}.$$
 (54)

In particular, the equal-time correlators yield the structure factor

$$S(k) \equiv \langle \gamma_k(t) \gamma_k^*(t) \rangle_c = \rho^{\text{eq}}(x), \tag{55}$$

which is independent of k.

dipolar diffusion

Based on the analysis for regular diffusion, it is tempting to guess that noise can be added to the dipolar diffusion equation simply by adding a term $\partial_i^2 \eta(t)$ where now $\eta_i(t)$ has autocorrelators equal to $2D\delta_{t,t'}\delta_{i,j}\rho_i^2(t)$. We will see that this is fact correct.

Specializing to 1d for simplicity, consider the $101 \leftrightarrow 020$ dipolar diffusion process generated by taking $\mathbf{a} = (1,3)$, $\mathbf{b} = (1,1)$. Following the same steps as in the analysis for regular diffusion (and being a bit more laconic now that we know how things work), we find

$$\ln W[\hat{\Gamma}] = r \sum_{i,t} \left(\rho_{i-1}(t) \rho_{i+1}(t) (e^{-\partial_i^2 \Gamma_i(t)} - 1) + \rho_i(t)^2 (e^{\partial_i^2 \Gamma_i(t)} - 1) \right).$$
 (56)

Taking one functional derivative and sending $\hat{\Gamma} \to 0$ gives

$$\partial_t \rho_i = \partial_i^2 \frac{\delta \ln W[\hat{\Gamma}]}{\delta \partial_i^2 \Gamma_i(t)} = D \partial_i^2 (\rho_i^2(t) - \rho_{i-1}(t) \rho_{i+1}(t)), \tag{57}$$

with the the expression in parenthesis correctly becoming $(\partial \rho)^2 - \rho \partial^2 \rho$ in the continuum limit.

Taking two functional derivatives on the other hand gives

$$\langle \partial_t \rho_i \partial_{t'} \rho_j \rangle_c = 2D \delta_{t,t'} \partial_i^2 \partial_j^2 (\rho_i(t)^2 \delta_{i,j}), \tag{58}$$

where we have dropped higher derivatives of the density. Note that we correctly have $\sum_{i} i^{m} \langle \partial_{t} \rho_{i} \partial_{t'} \rho_{j} \rangle_{c} = \sum_{j} j^{m} \langle \partial_{t} \rho_{i} \partial_{t'} \rho_{j} \rangle_{c}$ for m = 0, 1, 2. We also see that we may thus write the Langevin equation as

$$\partial_t \rho = D\partial^2((\partial \rho)^2 - \rho \partial^2 \rho) + \partial^2 \eta, \tag{59}$$

where now the noise field has autocorrelators

$$\langle \eta_i(t)\eta_i(t')\rangle_c = 2D\delta_{t,t'}\delta_{i,j}\rho_i^2(t). \tag{60}$$

As before, we can use the Langevin equation to derive the structure factor for the density fluctuations about local equilibirum. We again write $\rho(x,t) = \rho^{\rm eq}(x) + \gamma(x,t)$, but the nonlinearity of the dipolar diffusion equation forces us to make an additional assumption, namely that gradients of $\rho^{\rm eq}$ are all much smaller than $\rho^{\rm eq}$ itself. Even though $\rho^{\rm eq}$ is an exponential function of position in the present case, the length scale of this exponential is thermodynamically large as long as $x_{\rm cm}$ is. So as long as the center of mass $x_{\rm cm} = \omega(L^0)$, derivatives of $\rho^{\rm eq}$ can indeed be dropped. Then the linearized Langevin equation for γ reads

$$\gamma = -\frac{k^2}{i\omega + \tilde{D}k^4}\eta,\tag{61}$$

where the effective subdiffusion constant $\widetilde{D} \equiv D\rho^{eq}(x)$. Again assuming that ρ^{eq} is slowly varying to compute the η correctors, we obtain

$$\langle \gamma_{k\omega} \gamma_{k\omega}^* \rangle_c = 2\widetilde{D} \rho^{\text{eq}}(x) \frac{k^4}{\omega^2 + (\widetilde{D}k^4)^2}.$$
 (62)

Thus the structure factor is in fact exactly the same as in the case of conventional diffusion, viz.

$$S(k) = \rho^{\text{eq}}(x). \tag{63}$$

quantum multipolar diffusion

It is straightforward to understand the equilibirum states that occur for multipole-conserving quantum particles; all one has to do is replace classical distinguishible particles with bosons or fermions, as appropriate. For simplicity we will mostly consider dipole conserving particles in 1d box, $x \in [-L/2, L/2]$. As before we will let $N \equiv Q^{(0)}$, $x_{\rm cm} \equiv Q^{(1)}/N$.

fermions

Denote the Lagrange multiplier for dipole moment as β , and the multiplier for total charge as $-\beta\mu$. Then

$$N = \int_{-L/2}^{L/2} \frac{dx}{e^{\beta(x-\mu)} + 1} \implies \mu = \frac{1}{\beta} \ln \left(\frac{e^{\beta L/2} - e^{\beta N}}{e^{\beta N} - e^{\beta L}} \right). \tag{64}$$

The analogous equation for $x_{\rm cm}$ is rather complicated, and the explicit expression involves polylogarithms. Thus we specify to the simple case of half-filling, where N=L/2. This forces $\mu=0$, with $x_{\rm cm}$ then determining the effective "temperature": high T corresponds to $x_{\rm cm}=0$, while $T=0^+$ corresponds to $x_{\rm cm}=-L/4$ and $T=0^-$ has $x_{\rm cm}=+L/4$.

Various cute things are possible when we consider higher multipole moments. For example, consider an infinite system with quadrupole moment conservation. Then the

equilibrium state is a "Fermi surface" in real space: taking $Q_a^{(2)}$ to be independent of a for simplicity (so that the FS is spherical), the FS "radius" is then roughly fixed by the total number of particles, while the temperature is determined by the size of $Q^{(2)}$.

bosons

Now we discuss the bosonic case. First consider a dipole conserving system in finite box of size $[0, L]^d$. The interesting question to ask is when a "real space BEC" occurs, with all of the bosons spontaneously condensing at a given spatial point.

A BEC will occur when $\mu \to 0$, which means (assuming equal dipole moments along all spatial directions for simplicity)

$$N = \int_{\mathbb{R}^d} \frac{d^d r}{e^{\beta_* \sum_a r_a} - 1} \implies T_* = \left(N^{-1} \int_0^{\beta_* L} \frac{d^d r}{e^{\sum_a r_a} - 1} \right)^{-1/d}. \tag{65}$$

The integral on the RHS has a UV divergence (in the conventional Bose gas context for BECs, the role of position is swapped with that of momentum, and it is instead an IR divergence) when d = 1, but is finite when d > 1. Assuming that $\beta_* L = \Omega(L^0)$, in d > 1 we then have

$$T_* \propto N^{1/d},\tag{66}$$

so that our assumption $\beta_* L = \Omega(L^0)$ is satisfied if we are at fillings $N/L^d = O(L^0)$.

We now ask to what dipole moment this temperature corresponds to. This is determined by

$$Q^{(1)} = T_*^{d+1} \int_0^{\beta_* L} d^d r \frac{r}{e^{\sum_a r_a} - 1},$$
(67)

with the integral UV-finite in all dimensions. Thus

$$T_* \propto (Q^{(1)})^{1/(1+d)},$$
 (68)

and so the transition occurs when the center of mass $x_{\rm cm} = D/N$ satisfies

$$x_{\rm cm} \le CN^{1/d} \tag{69}$$

where here and below C will be used to denote unimportant numerical constants. Thus the transition occurs when $x_{\rm cm}$ is thermodynamically large

Consider now a quadrupole conserving system in infinite volume. The condition for a BEC to occur reads

$$N = \int \frac{d^d r}{e^{\beta_* r^2} - 1} \implies \beta_*^{d/2} N = S^{(d-1)} \int_0^\infty dr \frac{r^{d-1}}{e^{r^2} - 1}.$$
 (70)

The integral on the RHS is finite if d > 2, for $d \le 2$ it has a UV divergence. When d > 2 we thus get a critical temperature that goes as

$$T_* \propto N^{2/d}.\tag{71}$$

More meaningful is the quadrupole moment to which this temperature corresponds. Assuming rotational invariance for simplicity, this quadrupole moment is

$$Q_a^{(2)} = \frac{1}{d} \int dr \frac{r^{d+1}}{e^{\beta r^2} - 1} = CT_*^{1+d/2}.$$
 (72)

Thus using the above scaling for T_* , we see that a BEC forms when the quadrupole moment

$$Q_a^{(2)} \le CN^{1+2/d},\tag{73}$$

which is parametrically much smaller than its maximum value $Q_{a,max}^{(2)} \propto N^{2+d}$. The standard deviation of the particles is $\sigma = \sqrt{N^{-1}Q^{(2)}}$, so that a BEC forms when the standard deviation satisfies

$$\sigma < CN^{1/d},\tag{74}$$

which has the same scaling as the critical center of mass in the dipole conserving case. In fact this is not a conincidence, and it is easy to check that the condition for a BEC to form in general is that

$$l_*^{(n)} = O(N^{1/d}), \qquad d > n, \qquad N = O(L^d),$$
 (75)

where

$$l_*^{(n)} \equiv (Q^{(n)}/N)^{1/n}. (76)$$

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