IOP Publishing New J. Phys. 26 (2024) 013040 https://doi.org/10.1088/1367-2630/ad17d9

New Journal of Physics
The open access journal at the forefront of physics

Deutsche Physikalische Gesellschaft DPG
IOP Institute of Physics
Published in partnership with: Deutsche Physikalische Gesellschaft and the Institute of Physics

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OPEN ACCESS

RECEIVED
26 December 2022

REVISED
27 November 2023

ACCEPTED FOR PUBLICATION
21 December 2023

PUBLISHED
22 January 2024

PAPER

Field theory of active Brownian particles in potentials

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Keywords: active Brownian particles, active matter, Mathieu function

Abstract

The active Brownian particle (ABP) model exemplifies a wide class of active matter particles. In this work, we demonstrate how this model can be cast into a field theory in both two and three dimensions. Our aim is manifold: we wish both to extract useful features of the system, as well as to build a framework which can be used to study more complex systems involving ABPs, such as those involving interaction. Using the two-dimensional model as a template, we calculate the mean squared displacement exactly, and the one-point density in an external potential perturbatively. We show how the effective diffusion constant appears in the barometric density formula to leading order, and determine the corrections to it. We repeat the calculation in three dimensions, clearly a more challenging setup. Comparing different ways to capture the self-propulsion, we find that its perturbative treatment results in more tractable derivations without loss of exactness, where this is accessible.

1. Introduction

Active Brownian particles (ABPs) [1] are one of the paradigmatic models of active matter [2]. Such particles move with a constant self-propulsion *speed* w_0, in a time-varying direction, represented by a vector subject to rotational diffusion with constant D_r. At the same time, the particles are subject to thermal diffusion with constant D_t [3, 4]. As opposed to run-and-tumble (RnT) motion [3], both degrees of freedom, the vectorial velocity $\mathbf{w}(t)$ as well as the position $\mathbf{r}(t)$, are continuous functions of time t. ABPs approximate so-called Janus particles particularly well [1, 2]. Similarly, *monotrichous* bacteria vary their orientation more smoothly and are much more reliant on rotational diffusion [5]. In contrast, the motion of the much-studied *E. coli* is closer to RnT [6, 7].

The motion of ABPs is most directly described by a pair of Langevin equations for their position $\mathbf{r}(t)$ as a function of time t,

$$\partial_t \mathbf{r}(t) = \mathbf{w}(t) + \boldsymbol{\xi}(t) \quad \text{with} \quad \left\langle \boldsymbol{\xi}(t)\boldsymbol{\xi}^\mathsf{T}(t')\right\rangle = 2\mathsf{D}_t \mathbb{1}_d \delta(t'-t) \tag{1a}$$

$$\partial_t \mathbf{w}(t) = \boldsymbol{\zeta}_{\perp \mathbf{w}(t)}(t) \quad \text{with} \quad \left\langle \boldsymbol{\zeta}_{\perp \mathbf{w}(t)}(t)\cdot\boldsymbol{\zeta}_{\perp \mathbf{w}(t')}(t')\right\rangle = 2(d-1)\, w_0^2 \mathsf{D}_r \delta(t'-t) \tag{1b}$$

where the angular brackets $\langle \bullet \rangle$ indicate an ensemble average. Both $\boldsymbol{\xi}(t)$ and $\boldsymbol{\zeta}_{\perp \mathbf{w}(t)}(t)$ represent white noise with vanishing mean and correlators as stated, where $\left\langle \boldsymbol{\xi}(t)\boldsymbol{\xi}^\mathsf{T}(t')\right\rangle$ denotes the outer product and $\mathbb{1}_d$ the d-dimensional identity matrix. The translational noise $\boldsymbol{\xi}(t)$ is the commonly used Gaussian displacement in d dimensions. As there are no cross-correlations, the dot-product of the noise produces the characteristic $\langle \boldsymbol{\xi}(t)\cdot\boldsymbol{\xi}(t')\rangle = 2d\mathsf{D}_t\delta(t'-t)$. The rotational noise $\boldsymbol{\zeta}_{\perp \mathbf{w}(t)}(t)$ is confined to the $(d-1)$-dimensional tangential plane orthogonal to $\mathbf{w}(t)$ at any time [8], so that $\mathbf{w}(t)$ stays on the surface of a sphere of radius w_0

at any time. This is guaranteed by demanding $\langle \mathbf{w}(t) \cdot \boldsymbol{\zeta}_{\perp \mathbf{w}(t)}(t) \rangle = 0$ and by specifying that equation (1b) is subject to an Ito interpretation, in order to make the definition of the rotational noise precise. In section 1.1 we cast the above in Fokker–Planck form, avoiding any such issues of stochastic calculus.

The motion of ABPs in two dimensions has been analysed in various ways using classical methods [2–4, 9, 10], while ABPs in three dimensions have received much less attention. This might be related to the complications arising from the curvature of the surface the rotational diffusion takes place on. The aim of the present work is to develop the mathematical toolkit that will allow us to study ABPs using field theory. Some of us have studied ABPs in two dimensions before [11]. We will now study ABPs in two dimensions from a different perspective, primarily to provide us with a template for the treatment in three dimensions.

Studying ABPs in two and three dimensions through field theory will not only give direct insight about ABPs—developing and verifying this framework will also open the door to add interaction. We take a first step in this work by considering external potentials. Adding to this, say, pair-interaction equation (10), is solely a matter of adding a further term to this action [12–14], and similarly for adding reactions [15–17] or an external potential [11, 18]. The purpose of the present work is to characterise the basic framework which can serve as the foundation for more complicated systems, such as the Vicsek Model [12, 13, 19–21]. Similarly, replacing diffusive particles in well-understood particle systems by ABPs, is solely a matter of replacing, in a suitable representation, the bare propagators by those discussed in the following.

In the present work, we use Doi–Peliti field theory [15, 22–25] as the tool to characterise particle dynamics. Doi–Peliti field theory allows Fokker–Planck-equations and master equations [12] to be cast in a field theory without compromising particle entity [18]. This is a built-in feature, that has to be enforced 'by hand' by a Dean-term [26] in the more commonly used the response-field formalism [25, 27–29].

There are, in principle, always two ways of describing single-particle dynamics using Doi–Peliti field theory. Either, one can use a suitable eigensystem in which to expand the fields, or proceed by considering the motion as a perturbation about pure diffusion. The former approach is, in theory, more powerful, as the particle dynamics is fully contained in a set of eigenfunctions, whose eigenvalues determine the 'decay' rates. However, a combination of the two approaches is sometimes called for, particularly when there are multiple intertwined degrees of freedom, not all of which can be included in an appropriate eigensystem. The motion of RnT particles in a harmonic potential is an example of such a system [30] and similarly boundary tumbling [31]. In the present case of ABPs, the choice seems obvious in two dimensions, as, after suitable simplifications and without the need of any approximations, we encounter the Mathieu equation, whose eigenfunctions [32, 33] are well-known and have featured in related models, such as the worm-like chain model [34, 35]. However, in three dimensions, no such simplifications are available and the eigenfunctions not commonly used. This necessitates exploring new methods, in particular determining the eigenfunctions themselves perturbatively, or treating self-propulsion as a perturbation about pure diffusion. This latter method is first tried out in the easier case of two dimensions.

The complexity of the methods increases further when we allow for an external potential, which must be treated perturbatively. As a test bed for the methods, we return to ABPs in two dimensions [11], before moving on to three dimensions. In both cases, we determine the mean squared displacement (MSD) in closed form, as well as the stationary density in the presence of an external potential. These two observables are related: the MSD naturally gives rise to the notion of an *effective diffusion constant*, which may or may not feature as the effective temperature in a Boltzmann-like distribution of particles in the stationary state. ABPs have been studied in a range of setups [36, 37], including a harmonic trap [38]. In the present work, we aim to provide a general, but perturbative expression for the particle density.

The density of ABPs in potentials thus provides some new, original insight into their dynamics and statistics, whereas the calculation of the well-known MSD [3, 4, 11, 39] serves mainly the purpose of a sanity check of our framework. Calculating both observables gives us an opportunity to validate and assess the advantages and disadvantages of the different methods considered.

In the following, we introduce the ABP model, first through a Fokker–Planck description, and subsequently in the form of an action. In section 2, we proceed to characterise the MSD and stationary distribution in two dimensions. We do this first using Mathieu functions, and then perturbatively. These methods and results serve as the template for the treatment of ABPs in three dimensions in section 3.

1.1. ABPs

ABPs are particles that move by self-propulsion by a constant speed w_0 as well as due to thermal noise characterised by translational diffusion constant D_t. The direction of the self-propulsion is itself subject to diffusion. In the following, we will generally denote this direction by Ω, and more specifically in the plane the polar angle by $\varphi \in [0, 2\pi)$ and in spherical coordinates the azimuthal angle by $\varphi \in [0, 2\pi)$ and the polar angle by $\theta \in [0, \pi)$. The direction of the self-propulsion is then

$$\mathbf{w}(\Omega) = \begin{pmatrix} w_x \\ w_y \end{pmatrix} = w_0 \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix} \quad \text{and} \quad \mathbf{w}(\Omega) = \begin{pmatrix} w_x \\ w_y \\ w_z \end{pmatrix} = w_0 \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix} \tag{2}$$

in two and three dimensions respectively. The rotational diffusion is parameterised by the constant D_r, specifically by a Fokker-Planck equation of the form $\partial_t P(\Omega, t) = \mathsf{D}_r \nabla^2_\Omega P(\Omega, t)$ with

$$\nabla^2_\Omega = \partial^2_\varphi \quad \text{and} \quad \nabla^2_\Omega = \frac{1}{\sin\theta}\partial_\theta \sin\theta\, \partial_\theta + \frac{1}{\sin^2\theta}\partial^2_\varphi \tag{3}$$

in two and three dimensions respectively.

The Fokker–Planck equation of ABPs is

$$\partial_t P(\mathbf{r}, \Omega, t) = \mathcal{L} P(\mathbf{r}, \Omega, t) \quad \text{with} \quad \mathcal{L} = \mathsf{D}_t \nabla^2_\mathbf{r} - \mathbf{w}(\Omega)\cdot\nabla_\mathbf{r} + \nabla_\mathbf{r}\cdot(\nabla_\mathbf{r}\Upsilon(\mathbf{r})) + \mathsf{D}_r\nabla^2_\Omega \tag{4}$$

where $P(\mathbf{r}, \Omega, t)$ is the probability to find a particle after some initialization at time t at position $\mathbf{r}$ with the director pointing to Ω and $\nabla_\mathbf{r}$ the usual spatial gradient as opposed to ∇_Ω acting on the director, equation (3). The self-propulsion is implemented by the term $\mathbf{w}\cdot\nabla_\mathbf{r}$, which is the only term mixing the degrees of freedom Ω and $\mathbf{r}$. The effect of an additional external potential $\Upsilon(\mathbf{r})$ which acts equally on particles without orientation is implemented by $\nabla_\mathbf{r}\cdot(\nabla_\mathbf{r}\Upsilon)$, which is structurally identical to that of a drift $\mathbf{w}$ and reduces to that term when $\nabla_\mathbf{r}\Upsilon$ is constant in space. We write Υ' for $\nabla_\mathbf{r}\Upsilon$ in the following. When the operator $\nabla_\mathbf{r}\cdot\Upsilon'$ acts on P in equation (4), only the leftmost spatial gradient $\nabla_\mathbf{r}$ acts on the product of Υ' and P, whereas $\nabla_\mathbf{r}\Upsilon$ results solely in Υ'. For ease of notation below, we further introduce

$$\mathcal{L}_1 = \mathsf{D}_t\nabla^2_\mathbf{r} - \mathbf{w}(\Omega)\cdot\nabla_\mathbf{r} + \mathsf{D}_r\nabla^2_\Omega \tag{5a}$$

$$\mathcal{L}_2 = \mathsf{D}_t\nabla^2_\mathbf{r} + \mathsf{D}_r\nabla^2_\Omega\,. \tag{5b}$$

From the single-particle Fokker–Planck equation (4) the multiple, non-interacting particle action

$$\mathcal{A}[\tilde{\chi}, \chi] = \int \mathrm{d}^d r \int \mathrm{d}\Omega \int \mathrm{d}t\, \tilde{\chi}(\mathbf{r}, \Omega, t)\left(-\partial_t + \mathcal{L} - \mu\right)\chi(\mathbf{r}, \Omega, t) \tag{6}$$

follows immediately [12], with an additional mass $\mu \downarrow 0$ as a regulator and where χ and $\tilde{\chi}$ are annihilation field and Doi-shifted creation fields respectively [15, 22]. The integrals over $\mathbf{r}$ and t are taken over the entire space $\mathbb{R}^d$ and time $\mathbb{R}$ respectively, e.g. $\int \mathrm{d}^2 r = \iint_{-\infty}^{\infty} \mathrm{d}^2 r$ and $\int \mathrm{d}t = \int_{-\infty}^{\infty} \mathrm{d}t$ unless specified differently, and similarly for the solid angle Ω, the integral $\int \mathrm{d}\Omega$ runs over a d-dimensional unit sphere. At this stage, we leave the dimension $d \in \{2, 3\}$ and the integral $\int \mathrm{d}\Omega$ unspecified. Expectations of the annihilator field $\chi(\mathbf{r}, \Omega, t)$ and the creator field $\tilde{\chi}(\mathbf{r}, \Omega, t)$ can be calculated in a path integral [12]

$$\langle \bullet \rangle = \int \mathcal{D}\chi \mathcal{D}\tilde{\chi} \bullet \mathrm{e}^{\mathcal{A}[\tilde{\chi}, \chi]} = \left\langle \bullet\, \mathrm{e}^{\mathcal{A}_P[\tilde{\chi}, \chi]} \right\rangle_0 \quad \text{with} \quad \langle \bullet \rangle_0 = \int \mathcal{D}\tilde{\chi}\mathcal{D}\chi \bullet \mathrm{e}^{\mathcal{A}_0[\tilde{\chi}, \chi]}\,, \tag{7}$$

which allows for a perturbative treatment by splitting the action $\mathcal{A} = \mathcal{A}_0 + \mathcal{A}_P$ into a harmonic part $\mathcal{A}_0$, whose path-integral is readily taken, and a perturbative part $\mathcal{A}_P$, whose exponential is expanded,

$$\langle \bullet \rangle = \int \mathcal{D}\chi \mathcal{D}\tilde{\chi}\, \mathrm{e}^{\mathcal{A}_0[\tilde{\chi}, \chi]} \bullet \sum_{n=0}^{\infty} \frac{\mathcal{A}_P^n}{n!} = \left\langle \bullet \sum_{n=0}^{\infty} \frac{\mathcal{A}_P^n}{n!} \right\rangle_0\,, \tag{8}$$

where we have introduced $\langle \bullet \rangle_0$ as an average on the basis of the harmonic part of the action only. As the radius of convergence of an exponential is infinite, smallness of $\mathcal{A}_P$ is in principle not required. However, the power series $\sum_n \langle \bullet \mathcal{A}_P^n \rangle_0 / n!$ that arises from equation (8) after exchanging expectation and summation generally does not have an infinite radius of convergence in the parameters. Below we will find that the resulting series for the MSD has only a finite number of non-vanishing terms, so that convergence is obvious. When we calculate the density in the presence of an external field, we will be content with the leading order corrections, i.e. the first few terms in the expansion.

Which part of the action equation (6) is treated perturbatively depends crucially on the eigensystem the fields χ and $\tilde{\chi}$ are written in, as it determines which part of the operator becomes diagonal. Because the external potential is arbitrary, it cannot be diagonalised in its present generality.

We may thus consider two schemes: In the first, the fields are written in eigenfunctions of $\mathcal{L}_1$, equation (5), with the harmonic and perturbative part of the action

$$\mathcal{A}_{01} = \int \mathrm{d}^d r \int \mathrm{d}\Omega \int \mathrm{d}t \, \tilde{\chi}(\mathbf{r},\Omega,t)\left(-\partial_t + \mathcal{L}_1 - \mu\right)\chi(\mathbf{r},\Omega,t) \tag{9a}$$

$$\mathcal{A}_{P1} = \int \mathrm{d}^d r \int \mathrm{d}\Omega \int \mathrm{d}t \, \tilde{\chi}(\mathbf{r},\Omega,t)\nabla_{\mathbf{r}} \cdot \left[\left(\nabla_{\mathbf{r}} \Upsilon(\mathbf{r})\right)\chi(\mathbf{r},\Omega,t)\right] , \tag{9b}$$

which is more efficiently dealt with using Gauss' theorem in $\mathcal{A}_{P1}$ to make $\nabla_{\mathbf{r}}$ act on $\tilde{\chi}$ rather than $\Upsilon'\chi$.

The benefit of including the self-propulsion in the harmonic part of the action $\mathcal{A}_{01}$, equation (9a), via $\mathcal{L}_1$, equation (5a), at the expense of having to find suitable eigenfunctions, is to have only one perturbative vertex to worry about, namely that representing the external potential.

The major disadvantage is that eigenfunctions that diagonalise $\mathcal{L}_1$ may render terms in the action that contain products beyond the bilinear $\tilde{\chi}\chi$, such as an external potential in the form $\tilde{\chi}\nabla_{\mathbf{r}} \cdot (\nabla_{\mathbf{r}}\Upsilon)\chi$, significantly messier. In the case of Fourier-eigenfunctions, this is due to an external potential breaking momentum-conservation. A related problem would be encountered if we were to allow for pair interaction, say [12, 13]

$$\mathcal{A}_{\text{inter}} = \int \mathrm{d}^d r \int \mathrm{d}\Omega \int \mathrm{d}t \, \tilde{\chi}(\mathbf{r},\Omega,t) \int \mathrm{d}^d r' \int \mathrm{d}\Omega' \, \chi(\mathbf{r}',\Omega',t)\left(1+\tilde{\chi}(\mathbf{r}',\Omega',t)\right)\nabla_{\mathbf{r}}\left(\nabla_{\mathbf{r}} U(\mathbf{r}-\mathbf{r}')\right)\chi(\mathbf{r},\Omega,t) \tag{10}$$

with pair-force $\nabla_{\mathbf{r}} U(\mathbf{r}-\mathbf{r}')$.

The eigenfunctions of the angular part of $\mathcal{L}_1$ in two spatial dimensions, after some manipulation, are the π-periodic Mathieu functions [33], as discussed further below. Compared to other orthonormal systems, they are far less well studied [32]. In three dimensions, we shall call them 'three-dimensional Mathieu functions', but as far as we are aware, they have not been introduced in the literature of orthonormal functions in their own right. We have characterised them to some extent in appendix A using similar tools as outlined in [33]. Of course, the complete framework of Sturm–Liouville theory provides broad theoretical backing.

Once the existence of the eigenfunctions is established, they need to be determined only to the extent required by the observables.

In the second scheme, the fields are written in terms of eigenfunctions of the simpler $\mathcal{L}_2$ in equation (5), with the harmonic and perturbative part of the action

$$\mathcal{A}_{02} = \int \mathrm{d}^d r \int \mathrm{d}\Omega \int \mathrm{d}t \, \tilde{\chi}(\mathbf{r},\Omega,t)\left(-\partial_t + \mathcal{L}_2 - \mu\right)\chi(\mathbf{r},\Omega,t) \tag{11a}$$

$$\mathcal{A}_{P2} = \int \mathrm{d}^d r \int \mathrm{d}\Omega \int \mathrm{d}t \, \tilde{\chi}(\mathbf{r},\Omega,t)\nabla_{\mathbf{r}} \cdot \left(\nabla_{\mathbf{r}} \Upsilon(\mathbf{r}) - \mathbf{w}(\Omega)\right)\chi(\mathbf{r},\Omega,t) . \tag{11b}$$

This results in simpler expressions overall, but suffers from the significant disadvantage of an additional vertex mediating the self-propulsion. One may expect a significantly enlarged number of diagrams to be considered in any interesting observable, but this is not the case for the observables considered here.

We proceed by determining the MSD and the stationary density for ABPs in two dimensions. In the course, we will discuss the details of the action, the diagrammatics and the eigenfunctions.

2. ABPs in two dimensions

2.1. Mathieu functions

The starting point of the present derivation is the operator $\mathcal{L}_1$ in equation (5a) and the action equation (9a), restated here with the explicit parameterisation of the director

$$\mathcal{A}_{01}[\tilde{\chi},\chi] = \int \mathrm{d}^2 r \int_0^{2\pi} \mathrm{d}\varphi \int \mathrm{d}t \, \tilde{\chi}(\mathbf{r},\varphi,t)\left(-\partial_t + \mathcal{L}_1 - \mu\right)\chi(\mathbf{r},\varphi,t) \tag{12}$$

for convenience. The key difficulty here is to find eigenfunctions of the operator $-\mathbf{w} \cdot \nabla_{\mathbf{r}} + \nabla_{\Omega}^2$. This is greatly helped by measuring the azimuthal angle relative to the reciprocal vector $\mathbf{k}$, as we will discuss in the following. Using the completeness of the relevant orthogonal systems, we first introduce

$$\chi(\mathbf{r},\varphi,t)=\int đ\omega đ^2k\sum_{\ell=0}^{\infty}\mathrm{e}^{-\mathring{\imath}\omega t}\mathrm{e}^{\mathring{\imath}\mathbf{k}\cdot\mathbf{r}}u_\ell\left(\frac{\varphi-\sigma(\mathbf{k})}{2},q(|\mathbf{k}|)\right)\chi_\ell(\mathbf{k},\omega) \tag{13a}$$

$$\tilde{\chi}(\mathbf{r},\varphi,t)=\int đ\omega đ^2k\sum_{\ell=0}^{\infty}\mathrm{e}^{-\mathring{\imath}\omega t}\mathrm{e}^{\mathring{\imath}\mathbf{k}\cdot\mathbf{r}}\tilde{u}_\ell\left(\frac{\varphi-\sigma(-\mathbf{k})}{2},q(|-\mathbf{k}|)\right)\tilde{\chi}_\ell(\mathbf{k},\omega) \tag{13b}$$

where $đk=\mathrm{d}^dk/(2\pi)^d$ and $đ\omega=\mathrm{d}\omega/(2\pi)$ and correspondingly, further down, $\bar{\delta}(\mathbf{k})=(2\pi)^d\delta(\mathbf{k})$ and $\bar{\delta}(\omega)=2\pi\delta(\omega)$ The functions $u_\ell(\gamma,q(k))$ and $\tilde{u}_\ell(\gamma,q(k))$ are suitably normalised π-periodic Mathieu functions [11, 32, 33], depending on the dimensionless, purely imaginary parameter

$$q(k)=\frac{2\mathring{\imath}w_0k}{\mathsf{D}_r} \tag{14}$$

which is a function of the (absolute) magnitude $k=|\mathbf{k}|=|-\mathbf{k}|$ of the $\mathbf{k}$ vector. The function $\sigma(\mathbf{k})$, hitherto undetermined, allows a crucial simplification of the action further below. The Mathieu functions are defined as the solutions of the eigenfunction equation (19) to be used below. For the time being it suffices to state orthogonality even in the presence of the shift by σ,

$$\bar{\delta}(\mathbf{k}+\mathbf{k}')\int_0^{2\pi}\mathrm{d}\varphi\,u_\ell\left(\frac{\varphi-\sigma(\mathbf{k})}{2},q(|\mathbf{k}|)\right)\tilde{u}_{\ell'}\left(\frac{\varphi-\sigma(-\mathbf{k}')}{2},q(|-\mathbf{k}'|)\right)=\bar{\delta}(\mathbf{k}+\mathbf{k}')\delta_{\ell,\ell'} \tag{15}$$

as the $\bar{\delta}(\mathbf{k}+\mathbf{k}')$ forces this shift to be identical, $\sigma(\mathbf{k})=\sigma(-\mathbf{k}')$, which can therefore be absorbed into the dummy variable and subsequently into a change of the integration limits, from where it disappears, because of the periodicity of the integrand. The orthogonality relation equation (15) together with the orthogonality of the Fourier modes

$$\int\mathrm{d}t\,\mathrm{e}^{-\mathring{\imath}\omega t}\mathrm{e}^{\mathring{\imath}\omega' t}=\bar{\delta}(\omega-\omega')\qquad\text{and}\qquad\int\mathrm{d}^dr\,\mathrm{e}^{-\mathring{\imath}\mathbf{k}\cdot\mathbf{r}}\mathrm{e}^{\mathring{\imath}\mathbf{k}'\cdot\mathbf{r}}=\bar{\delta}(\mathbf{k}-\mathbf{k}') \tag{16}$$

determines the reparameterised fields $\chi_\ell(\mathbf{k},\omega)$ and $\tilde{\chi}_\ell(\mathbf{k},\omega)$ in equation (13) uniquely from $\chi(\mathbf{r},\varphi,t)$ and $\tilde{\chi}(\mathbf{r},\varphi,t)$ respectively.

Using equation (13) in the action equation (12) produces

$$\mathcal{A}_{01}[\tilde{\chi},\chi]=-\int đ^2k\sum_{\ell,\ell'}\int đ\omega\,\tilde{\chi}_{\ell'}(-\mathbf{k},-\omega)\chi_\ell(\mathbf{k},\omega)\times\int_0^{2\pi}\mathrm{d}\varphi\,\tilde{u}_{\ell'}\left(\frac{\varphi-\sigma(\mathbf{k})}{2},q(k)\right)\left(-\mathring{\imath}\omega+\mathsf{D}_t\mathbf{k}^2+\mathring{\imath}w_0k\cos(\varphi-\alpha)-\mathsf{D}_r\partial_\varphi^2\right)u_\ell\left(\frac{\varphi-\sigma(\mathbf{k})}{2},q(k)\right), \tag{17}$$

where α is the polar angle of $\mathbf{k}=k(\cos\alpha,\sin\alpha)^\mathsf{T}$, so that $\mathbf{k}\cdot\mathbf{w}(\varphi)=kw(\cos\alpha\cos\varphi+\sin\alpha\sin\varphi)=kw\cos(\varphi-\alpha)$. Choosing $\sigma(\mathbf{k})=\alpha$ allows a change of variables and a change of integration limits, so that the last integral in equation (17) reads

$$\int_0^{2\pi}\mathrm{d}\varphi\,\tilde{u}_{\ell'}\left(\frac{\varphi-\sigma(\mathbf{k})}{2},q(k)\right)\left(-\mathring{\imath}\omega+\mathsf{D}_t\mathbf{k}^2+\mathring{\imath}w_0k\cos(\varphi-\alpha)-\mathsf{D}_r\partial_\varphi^2+\mu\right)u_\ell\left(\frac{\varphi-\sigma(\mathbf{k})}{2},q(k)\right) \tag{18a}$$

$$=2\int_0^{\pi}\mathrm{d}\gamma\,\tilde{u}_{\ell'}(\gamma,q)\left(-\mathring{\imath}\omega+\mathsf{D}_t\mathbf{k}^2+\frac{1}{4}\mathsf{D}_r\left(2q\cos(2\gamma)-\partial_\gamma^2\right)+\mu\right)u_\ell(\gamma,q) \tag{18b}$$

$$=\delta_{\ell',\ell}\left(-\mathring{\imath}\omega+\mathsf{D}_t\mathbf{k}^2+\frac{1}{4}\mathsf{D}_r\lambda_\ell(q)+\mu\right) \tag{18c}$$

where in the last equality we have used that the Mathieu functions obey

$$\left(\partial_\gamma^2-2q\cos(2\gamma)\right)u_\ell(\gamma,q)=-\lambda_\ell(q)u_\ell(\gamma,q) \tag{19}$$

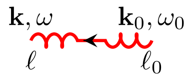
and the orthonormality equation (15).

With this simplification the action equation (12) becomes diagonal

$$\mathcal{A}_{01}[\tilde{\chi},\chi]=-\int đ^2k\sum_\ell\int đ\omega\,\tilde{\chi}_\ell(-\mathbf{k},-\omega)\chi_\ell(\mathbf{k},\omega)\left(-\mathring{\imath}\omega+\mathsf{D}_t\mathbf{k}^2+\mathsf{D}_r\lambda_\ell(q(k))/4+\mu\right), \tag{20}$$

and the (bare) propagator can immediately be read off

$$\langle \chi_\ell(\mathbf{k},\omega)\,\tilde{\chi}_{\ell_0}(\mathbf{k}_0,\omega_0)\rangle_0 = \frac{\delta_{\ell,\ell_0}\bar{\delta}\,(\mathbf{k}+\mathbf{k}_0)\,\bar{\delta}\,(\omega+\omega_0)}{-\mathring{\imath}\omega + \mathsf{D}_t\mathbf{k}^2 + \mathsf{D}_r\lambda_\ell(q(k))/4+\mu} = \delta_{\ell,\ell_0}\bar{\delta}\,(\mathbf{k}+\mathbf{k}_0)\,\bar{\delta}\,(\omega+\omega_0)\,G_\ell(\mathbf{k},\omega) \quad (21a)$$

$\triangleq$ 

, (21b)

where we have introduced $G_\ell(\mathbf{k},\omega)$ as a shorthand, as well as the diagrammatic representation to be used in section 2.1.2.

2.1.1. MSD

The MSD $\overline{\mathbf{r}^2}(t)$ of a two-dimensional ABP (2DABP) can be calculated on the basis of a few algebraic properties of the $u_\ell(\gamma,q)$. The probability of finding a 2DABP with director φ at position $\mathbf{r}$ at time t, after being placed at $\mathbf{r}_0$ with director φ_0 at time t_0 is $\langle\chi(\mathbf{r},\varphi,t)\tilde{\chi}(\mathbf{r}_0,\varphi_0,t_0)\rangle$, which is easily determined from equation (21) as

$$\langle\chi(\mathbf{k},\varphi,t)\tilde{\chi}(\mathbf{k}_0,\varphi_0,t_0)\rangle = \bar{\delta}\,(\mathbf{k}+\mathbf{k}_0)\sum_{\ell=0}^{\infty} u_\ell\left(\frac{\varphi-\sigma(\mathbf{k})}{2},q(k)\right)\tilde{u}_\ell\left(\frac{\varphi_0-\sigma(\mathbf{k})}{2},q(k)\right)\mathrm{e}^{-(\mathsf{D}_t k^2+\frac{1}{4}\mathsf{D}_r\lambda_\ell(q(k)))t} \quad (22)$$

up to an inverse of Fourier-transform of $\mathbf{k}$. Making use of the Fourier transform, the MSD of a 2DABP irrespective of the final director is

$$\overline{\mathbf{r}^2}(t) = -\left.\nabla^2_{\mathbf{k}}\right|_{\mathbf{k}=\mathbf{0}}\int_0^{2\pi}\mathrm{d}\varphi\sum_{\ell=0}^{\infty}u_\ell\left(\frac{\varphi-\sigma(\mathbf{k})}{2},q(k)\right)\tilde{u}_\ell\left(\frac{\varphi_0-\sigma(\mathbf{k})}{2},q(k)\right)\mathrm{e}^{-(\mathsf{D}_t k^2+\frac{1}{4}\mathsf{D}_r\lambda_\ell(q(k)))t}. \quad (23)$$

Having integrated over φ, it is obvious that the MSD cannot depend on the initial orientation of the director, φ_0, as changing it, amounts to a rotation of the isotropic plane. This is indeed trivial to show when $w_0=0$, in which case $q(k)=0$ and the Mathieu functions degenerate into trigonometric functions. However, demonstrating this when $w_0\neq 0$ is far from trivial. We proceed by rewriting the MSD as an average $\int\mathrm{d}\varphi_0\,(2\pi)^{-1}$ of equation (23) over the initial angle φ_0, so that both Mathieu functions, u_ℓ and $\tilde{u}_\ell$ reduce to a single coefficient via

$$\int_0^{2\pi}\mathrm{d}\varphi\,u_\ell(\varphi/2,q(k)) = 2\pi A_{\ell,0}(q(k))\,, \quad (24)$$

which vanishes in fact for all odd indices ℓ. We thus arrive at

$$\overline{\mathbf{r}^2}(t) = -\left.\nabla^2_{\mathbf{k}}\right|_{\mathbf{k}=\mathbf{0}}2\mathrm{e}^{-\mathsf{D}_t k^2 t}\sum_{\ell=0}^{\infty}(A_{\ell,0}(q(k)))^2\,\mathrm{e}^{-\frac{1}{4}\mathsf{D}_r\lambda_\ell(q(k))t}. \quad (25)$$

The $u_\ell(\gamma,q)$ are in fact the even π-periodic Mathieu functions for even ℓ and odd π-periodic Mathieu functions for odd ℓ [33].

The $\tilde{u}_\ell(\gamma,q)$ differ from the $u_\ell(\gamma,q)$ only by a factor $1/\pi$ [11],

$$\tilde{u}_\ell(\gamma,q) = \pi^{-1}u_\ell(\gamma,q)\,, \quad (26)$$

which is a convenient way to meet the orthogonality relation equation (15) while maintaining that the non-tilde $u_\ell(\gamma,q)$ are standard Mathieu functions. At this stage, all we need to know about the Mathieu functions is [33]

$$A_{0,0}(q) = \frac{1}{\sqrt{2}} - \frac{q^2}{16\sqrt{2}} + \mathcal{O}(q^3) \quad (27a)$$

$$A_{2,0}(q) = \frac{q}{4} + \mathcal{O}(q^2) \quad (27b)$$

$$A_{2j,0}(q) = \mathcal{O}(q^j) \quad (27c)$$

$$A_{2j+1,0}(q) = 0 \quad (27d)$$

$$\lambda_0 = \mathcal{O}(q^2) \quad (27e)$$

$$\lambda_2 = 4 + \mathcal{O}(q^2) \quad (27f)$$

for $j \in \mathbb{N}_0$, which means that only two of the $A_{\ell,0}$ in the sum equation (25) contribute, namely $\ell = 0$ and $\ell = 2$, as all other $A_{\ell,0}$ vanish at $q(k=0) = 0$ even when differentiated twice. With equation (27) the MSD becomes [11]

$$\overline{\mathbf{r}^2}(t) = 4\mathsf{D}_t t + 2\frac{w_0^2}{\mathsf{D}_r^2}\left(e^{-\mathsf{D}_r t} - 1 + \mathsf{D}_r t\right) , \tag{28}$$

identical to that of RnT particles, equation (49) of [11], if the tumble rate α is D_r. In asymptotically large t, the MSD of a 2DABP is equivalent to that of conventional diffusion with effective diffusion constant

$$\mathsf{D}_{\text{eff}}^{2\text{D}} = \mathsf{D}_t + \frac{w_0^2}{2\mathsf{D}_r} , \tag{29}$$

and RnT motion with tumbling rate $\alpha = \mathsf{D}_r$ [3, 4, 11].

We will use the above as a template for the derivation of the MSD of 3DABP. There, we will make use again of the isotropy of the initial condition φ_0 and further of the isotropy of the displacement in any of the three spatial directions. In fact, picking a 'preferred direction' can greatly reduce the difficulty of the present calculation.

2.1.2. External potential

Next, we place the 2DABP in a (two-dimensional) potential $\Upsilon(\mathbf{r})$. Without self-propulsion, the density $\rho_0(\mathbf{r})$ at stationarity is given by the barometric formula $\rho_0(\mathbf{r}) \propto \exp(-\Upsilon(\mathbf{r})/\mathsf{D}_t)$. As a sanity check for the present field-theoretic framework, we derive it in appendix C. In the present section we want to determine the effect of the self-propulsion, which we expect is partially covered by D_t in the Boltzmann distribution being replaced by $\mathsf{D}_{\text{eff}}^{2\text{D}}$, equation (29).

As the external potential is treated perturbatively, stationarity even at vanishing potential requires a finite volume, which we assume is a periodic square, i.e. a torus, with linear extent L. This requires a small adjustment of the Fourier representation introduced in equation (13), which now reads

$$\chi(\mathbf{r},\varphi,t) = \int đ\,\omega \frac{1}{L^2} \sum_{\mathbf{n}\in\mathbb{Z}^2} \sum_{\ell=0}^{\infty} \mathrm{e}^{-\imath\omega t} \mathrm{e}^{\imath\mathbf{k}_\mathbf{n}\cdot\mathbf{r}} u_\ell\left(\frac{\varphi - \sigma(\mathbf{k}_\mathbf{n})}{2}, q(|\mathbf{k}_\mathbf{n}|)\right) \chi_\ell(\mathbf{k}_\mathbf{n},\omega) \tag{30a}$$

$$\tilde{\chi}(\mathbf{r},\varphi,t) = \int đ\,\omega \frac{1}{L^2} \sum_{\mathbf{n}\in\mathbb{Z}^2} \sum_{\ell=0}^{\infty} \mathrm{e}^{-\imath\omega t} \mathrm{e}^{\imath\mathbf{k}_\mathbf{n}\cdot\mathbf{r}} \tilde{u}_\ell\left(\frac{\varphi - \sigma(-\mathbf{k}_\mathbf{n})}{2}, q(|-\mathbf{k}_\mathbf{n}|)\right) \tilde{\chi}_\ell(\mathbf{k}_\mathbf{n},\omega) \tag{30b}$$

where $L^{-2}\sum_{\mathbf{n}\in\mathbb{Z}^2}$ has replaced the integration over $\mathbf{k}$ in equation (13), with the couple $\mathbf{n} = (n_x, n_y)^\mathsf{T}$ running over the entire $\mathbb{Z}^2$ and $\mathbf{k}_\mathbf{n} = \mathbf{n}L/(2\pi)$. The bare propagator equation (21) is adjusted simply by replacing the Dirac δ-function in $\mathbf{k}$ by a Kronecker δ-function in the Fourier mode number, say $\delta\!\!\!{}^{-}(\mathbf{k}+\mathbf{k}_0)$ by, say, $L^2\delta_{\mathbf{n}+\mathbf{p},\mathbf{0}}$. With the introduction of Fourier sums, we implement periodic boundary conditions, effectively implementing periodic observables and, below, a periodic potential.

As far as the Mathieu functions are concerned this adjustment to a finite domain has no significant consequences. Due to the Mathieu functions, however, the perturbative part of the action $\mathcal{A}_{P1}$ equation (9b) gets significantly more difficult, as the functions are orthogonal only if the $\mathbf{k}$-modes match,

$$\mathcal{A}_{P1} = \int \mathrm{d}^d r \int \mathrm{d}\Omega \int \mathrm{d}t\, \tilde{\chi}(\mathbf{r},\Omega,t) \nabla_\mathbf{r} \cdot (\nabla_\mathbf{r}\Upsilon(\mathbf{r})) \chi(\mathbf{r},\Omega,t) \tag{31a}$$

$$= \int đ\,\omega \frac{1}{L^6} \sum_{\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3} L^2 \delta_{\mathbf{n}_1+\mathbf{n}_2+\mathbf{n}_3,\mathbf{0}} \sum_{\ell_1,\ell_3} (\mathbf{k}_{\mathbf{n}_1}\cdot\mathbf{k}_{\mathbf{n}_2}) \tilde{\chi}_{\ell_1}(\mathbf{k}_{\mathbf{n}_1},-\omega) \Upsilon_{\mathbf{n}_2} \chi_{\ell_3}(\mathbf{k}_{\mathbf{n}_3},\omega) \tag{31b}$$

$$\times \int_0^{2\pi} \mathrm{d}\varphi\, u_{\ell_3}\left(\frac{\varphi - \sigma(\mathbf{k}_{\mathbf{n}_3})}{2}, q(|\mathbf{k}_{\mathbf{n}_3}|)\right) \tilde{u}_{\ell_1}\left(\frac{\varphi - \sigma(-\mathbf{k}_{\mathbf{n}_1})}{2}, q(|\mathbf{k}_{\mathbf{n}_1}|)\right) \tag{31c}$$

where each $\mathbf{n}_1$, $\mathbf{n}_2$ and $\mathbf{n}_3$ runs over all $\mathbb{Z}^2$ in the sum and the Kronecker δ-function $\delta_{\mathbf{n}_1+\mathbf{n}_2+\mathbf{n}_3,\mathbf{0}}$ enforces $\mathbf{n}_1+\mathbf{n}_2+\mathbf{n}_3=\mathbf{0}$. Similarly, ℓ_1 and ℓ_3 run over all non-negative integers indexing the Mathieu functions. The potential $\Upsilon(\mathbf{r})$ now enters via its modes $\Upsilon_\mathbf{n}$, more explicitly

$$\Upsilon(\mathbf{r}) = \frac{1}{L^2}\sum_{\mathbf{n}\in\mathbb{Z}^2}\Upsilon_\mathbf{n}\mathrm{e}^{\mathring{\imath}\mathbf{k}_\mathbf{n}\cdot\mathbf{r}} \tag{32a}$$

$$\Upsilon_\mathbf{n} = \iint_0^L \mathrm{d}^2r\,\Upsilon(\mathbf{r})\,\mathrm{e}^{-\mathring{\imath}\mathbf{k}_\mathbf{n}\cdot\mathbf{r}}\,, \tag{32b}$$

rendering the potential effectively periodic.

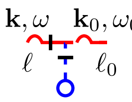
Of course, a non-trivial $\Upsilon(\mathbf{r})$ spoils translational invariance and correspondingly $\Upsilon_\mathbf{n}$ provides a *source* of momentum in equation (31*b*), so that $\mathbf{k}_{\mathbf{n}_3}$ is generally not equal to $-\mathbf{k}_{\mathbf{n}_1}$, with the sole exception of $\mathbf{n}_2=\mathbf{0}$. As a result, generally $\sigma(\mathbf{k}_{\mathbf{n}_3})\neq\sigma(-\mathbf{k}_{\mathbf{n}_1})$ and $q(|\mathbf{k}_{\mathbf{n}_3}|)\neq q(|\mathbf{k}_{\mathbf{n}_1}|)$, equation (14). The integral

$$\Delta_{\ell_1,\ell_3}(-\mathbf{k}_{\mathbf{n}_1},-\mathbf{k}_{\mathbf{n}_3}) = \int_0^{2\pi}\mathrm{d}\varphi\,u_{\ell_3}\left(\frac{\varphi-\sigma(\mathbf{k}_{\mathbf{n}_3})}{2},q(|\mathbf{k}_{\mathbf{n}_3}|)\right)\tilde{u}_{\ell_1}\left(\frac{\varphi-\sigma(-\mathbf{k}_{\mathbf{n}_1})}{2},q(|\mathbf{k}_{\mathbf{n}_1}|)\right) \tag{33}$$

however, is generally diagonal in ℓ_1,ℓ_3 only when $\mathbf{k}_{\mathbf{n}_1}=-\mathbf{k}_{\mathbf{n}_3}$, referred to above as 'matching $\mathbf{k}$-modes'. It is this projection, equation (33), that is at the heart of the complications to come. It is notably absent in the case of purely diffusive particles, appendix C.4. With the help of equation (33), the perturbative action equation (31*b*) can be written as

$$\mathcal{A}_{P1} = \int đ\,\omega\frac{1}{L^6}\sum_{\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3}L^2\delta_{\mathbf{n}_1+\mathbf{n}_2+\mathbf{n}_3,\mathbf{0}}\sum_{\ell_1,\ell_3}(\mathbf{k}_{\mathbf{n}_1}\cdot\mathbf{k}_{\mathbf{n}_2})\tilde{\chi}_{\ell_1}(\mathbf{k}_{\mathbf{n}_1},-\omega)\Upsilon_{\mathbf{n}_2}\chi_{\ell_3}(\mathbf{k}_{\mathbf{n}_3},\omega)\Delta_{\ell_1,\ell_3}(-\mathbf{k}_{\mathbf{n}_1},-\mathbf{k}_{\mathbf{n}_3})\,. \tag{34}$$

The perturbative part of the action, equation (31*b*), may diagrammatically be written as



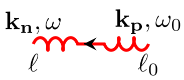
, (35)

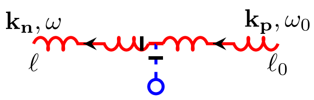
where a dash across any line serves as a reminder that the vertex carries a factor of $\mathbf{k}$ carried by the leg. Unless there are further singularities in $\mathbf{k}$, any such line vanishes at $\mathbf{k}=\mathbf{0}$. The two factors of $\mathbf{k}$ are multiplied in an inner product. The dangling bauble in equation (35) represents the external potential, which is a source of momentum.

We will determine in the following the stationary density

$$\rho_0(\mathbf{r}) = \lim_{t_0\to-\infty}\int_0^{2\pi}\mathrm{d}\varphi\,\langle\chi(\mathbf{r},\varphi,t)\,\tilde{\chi}(\mathbf{r}_0,\varphi_0,t_0)\rangle \tag{36}$$

at position $\mathbf{r}$, starting with a single particle placed at $\mathbf{r}_0$ with orientation φ_0 at time t_0. We will determine this density to first order in the potential and second order in $q=2\mathring{\imath}w_0k/\mathsf{D}_r$, equation (14), starting from the diagrammatic representation in inverse space,

$\langle\chi(\mathbf{k_n},\ell,\omega)\tilde{\chi}(\mathbf{k_p},\ell_0,\omega_0)\rangle \triangleq$ 

$+$ 

$+\dots\,,$ (37)

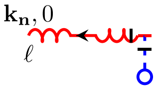
where the first diagram represents the bare propagator as introduced in equation (21) and the second diagram the contribution to first order due to the external potential equation (35). The limit $t_0\to-\infty$ needs to be taken after an inverse Fourier transform in ω and ω_0. The structure of the propagator equation (21), essentially of the form $(-\mathring{\imath}\omega+\lambda+\mu)^{-1}$ with some non-negative $\lambda\geqslant0$ dependent on the spatial and angular modes, means that every such Fourier transform results in an expression proportional to $\exp(-(\lambda+\mu)(t-t_0))$. Removing the mass by $\mu\downarrow0$ and taking $t_0\to-\infty$ results in the expression vanishing, except when $\Re(\lambda)\leqslant0$ [40], which is the case, by inspection of equation (21), only when $\mathbf{k}=\mathbf{0}$ and $\Re(\lambda_\ell(q(\mathbf{k})))\leqslant0$, which requires $\ell=0$, as

$$\lambda_{2\ell}(q) = 4\ell^2+\mathcal{O}(q)\,, \tag{38a}$$

$$\lambda_{2\ell+1}(q) = 4(\ell+1)^2+\mathcal{O}(q)\,. \tag{38b}$$

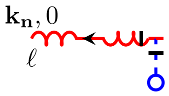
Equation (38) is easily verified as the periodic solutions of the Mathieu equation (19) are trigonometric functions. Any propagator carrying a factor of $\mathbf{k}$ therefore vanishes under this operation. The only pole of the propagator to be considered is the one at $\omega = -\imath\mu$. Because only the rightmost, incoming leg in any of the diagrams is undashed, taking the inverse Fourier transform followed by the limit $t_0 \to -\infty$ thus amounts to replacing the incoming legs by $\delta_{\mathbf{n},0}$ and every occurrence of ω in the diagram by 0. This is equivalent to an amputation of the incoming leg [40]. At this point, the inverse Fourier transforms from $\mathbf{k}$ to $\mathbf{r}$ and the transforms of azimuthal degree of freedom from ℓ to φ are still to be taken.

We may summarise by writing

$$\lim_{t_0\to-\infty} \langle \chi(\mathbf{k_n},\ell,t)\tilde{\chi}(\mathbf{k_p},\ell_0,t_0)\rangle \triangleq \delta_{\ell,\ell_0}\delta_{\ell_0,0}L^2\delta_{\mathbf{n+p},0}\delta_{\mathbf{p},\mathbf{0}} +$$ 

$$\times \left\{\delta_{\ell_0,0}\delta_{\mathbf{p},\mathbf{0}}\right\} + \ldots . \tag{39}$$

Using equations (21) and (34), the last diagram evaluates to



$$\times \left\{\delta_{\ell_0,0}\delta_{\mathbf{p},\mathbf{0}}\right\} = (-\mathbf{k_n}\cdot\mathbf{k_{n+p}})\Upsilon_{\mathbf{n+p}}G_\ell(\mathbf{k_n},0)\,\delta_{\ell_0,0}\delta_{\mathbf{p},\mathbf{0}}\Delta_{\ell,\ell_0}(\mathbf{k_n},\mathbf{k_p}) \tag{40}$$

The projection $\Delta_{\ell,\ell_0}(\mathbf{k_n},\mathbf{k_p})$ needs to be known only for $\ell_0 = 0$ and $\mathbf{k_p} = \mathbf{0}$, and because $u_{\ell=0}(\gamma, q=0) = 1/\sqrt{2}$, equations (24) and (33) give

$$\Delta_{\ell,0}(\mathbf{k_n},\mathbf{0}) = \sqrt{2}A_{\ell,0}(q(|\mathbf{k_n}|)) . \tag{41}$$

To carry out the integral over φ in equation (36), we have to transform equation (39) from ℓ,ℓ_0 to φ,φ_0 using equation (13) first,

$$\begin{aligned}
&\lim_{t_0\to-\infty}\left\langle \chi(\mathbf{k_n},\varphi,t)\,\tilde{\chi}(\mathbf{k_p},\varphi_0,t_0)\right\rangle \\
&= u_0\left(\frac{\varphi-\sigma(\mathbf{k_n})}{2}, q(|\mathbf{k_n}|)\right)\widetilde{u}_0\left(\frac{\varphi_0-\sigma(-\mathbf{k_p})}{2}, q(|\mathbf{k_p}|)\right)L^2\delta_{\mathbf{n+p},0}\delta_{\mathbf{p},\mathbf{0}} \\
&\quad + \sum_{\ell=0}^{\infty}(-\mathbf{k_n}\cdot\mathbf{k_{n+p}})\,\Upsilon_{\mathbf{n+p}}G_\ell(\mathbf{k_n},0)\,\delta_{\mathbf{p},\mathbf{0}}\sqrt{2}A_{\ell,0}(q(|\mathbf{k_n}|))\,u_\ell\left(\frac{\varphi-\sigma(\mathbf{k_n})}{2}, q(|\mathbf{k_n}|)\right) \\
&\quad \times \widetilde{u}_0\left(\frac{\varphi_0-\sigma(-\mathbf{k_p})}{2}, q(|\mathbf{k_p}|)\right) + \ldots .
\end{aligned} \tag{42}$$

In the first term, $\mathbf{k_n} = \mathbf{k_p} = \mathbf{0}$, so that the product of the two Mathieu functions degenerates to $1/(2\pi)$, cancelling with the integration over φ still to be performed. In the second term, integration over φ can again be done with the help of equation (24), while the final Mathieu function $\widetilde{u}_0(\frac{\varphi_0-\sigma(-\mathbf{k_p})}{2}, q(|\mathbf{k_p}|))$ is in fact $1/(\sqrt{2}\pi)$, once $\mathbf{k_p} = \mathbf{0}$ is taken into account,

$$\begin{aligned}
&\int_0^{2\pi}\mathrm{d}\varphi \lim_{t_0\to-\infty}\left\langle \chi(\mathbf{k_n},\varphi,t)\,\tilde{\chi}(\mathbf{k_p},\varphi_0,t_0)\right\rangle \\
&\quad = L^2\delta_{\mathbf{n+p},0}\delta_{\mathbf{p},\mathbf{0}} + \sum_{\ell=0}^{\infty}(-\mathbf{k_n}\cdot\mathbf{k_{n+p}})\,\Upsilon_{\mathbf{n+p}}G_\ell(\mathbf{k_n},0)\,\delta_{\mathbf{p},\mathbf{0}}2\left(A_{\ell,0}(q(|\mathbf{k_n}|))\right)^2 + \ldots .
\end{aligned} \tag{43}$$

Since $A_{\ell,0}(q)$, equation (27), vanish for odd ℓ and otherwise behave to leading order like $q^{\ell/2}$, equation (27), expanding these coefficients to second order means to retain only $\ell = 0, 2$ in the sum, so that with explicit $G_\ell(\mathbf{k_n}, 0)$, equation (21), we arrive at

$$\begin{aligned}
&\int_0^{2\pi}\mathrm{d}\varphi \lim_{t_0\to-\infty}\left\langle \chi(\mathbf{k_n},\varphi,t)\,\tilde{\chi}(\mathbf{k_p},\varphi_0,t_0)\right\rangle = L^2\delta_{\mathbf{n+p},0}\delta_{\mathbf{p},\mathbf{0}} + (-\mathbf{k_n}\cdot\mathbf{k_{n+p}})\,\Upsilon_{\mathbf{n+p}}\delta_{\ell_0,0}\delta_{\mathbf{p},\mathbf{0}} \\
&\quad \times\left\{\left(\mathsf{D}_t k_\mathbf{n}^2 + \mathsf{D}_r\lambda_0(q)/4+\mu\right)^{-1}\left(1-\frac{q^2}{16}\right)^2 + \left(\mathsf{D}_t k_\mathbf{n}^2 + \mathsf{D}_r\lambda_2(q)/4+\mu\right)^{-1}\frac{q^2}{8}\right\} + \mathcal{O}(q^4) + \ldots ,
\end{aligned} \tag{44}$$

where $q^2 = -4w_0^2k_{\mathbf{n}}^2\mathsf{D}_r^{-2}$ and $k_{\mathbf{n}} = |\mathbf{k}_{\mathbf{n}}|$. The limit $\mu\downarrow 0$ is yet to be taken and ... on the right of equation (44) refers to the higher orders in the external potential. Expanding the eigenvalues λ_ℓ beyond equation (27),

$$\lambda_0 = -q^2/2 + \mathcal{O}(q^4) = 2w_0^2k_{\mathbf{n}}^2\mathsf{D}_r^{-2} + \mathcal{O}(q^4) \tag{45a}$$

$$\lambda_2 = 4 + \mathcal{O}(q^2) \ , \tag{45b}$$

suggests that $\mathbf{k}_{\mathbf{n}}\cdot\mathbf{k}_{\mathbf{n}+\mathbf{p}}\delta_{\mathbf{p},\mathbf{0}}$ can be cancelled with $k_{\mathbf{n}}^2$ in the denominator when $\ell = 0$. However, for $\mathbf{n} = \mathbf{0}$ the denominator does not vanish as $\mu > 0$. Performing the inverse Fourier transform to return real space gives after $\mu\downarrow 0$,

$$\begin{aligned}\rho_0(\mathbf{r}) &= \frac{1}{L^4}\sum_{\mathbf{n},\mathbf{p}} \mathrm{e}^{\imath(\mathbf{k}_{\mathbf{n}}\cdot\mathbf{r}+\mathbf{k}_{\mathbf{p}}\cdot\mathbf{r}_0)}\int_0^{2\pi}\mathrm{d}\varphi \lim_{t_0\to-\infty}\left\langle\chi(\mathbf{k}_{\mathbf{n}},\varphi,t)\tilde{\chi}(\mathbf{k}_{\mathbf{p}},\varphi_0,t_0)\right\rangle \\ &= L^{-2} - \frac{1}{L^4}\sum_{\mathbf{n}\neq\mathbf{0}}\mathrm{e}^{\imath\mathbf{k}_{\mathbf{n}}\cdot\mathbf{r}}\Upsilon_{\mathbf{n}}\left\{\left(\mathsf{D}_t + w_0^2/(2\mathsf{D}_r) + \mathcal{O}(q^4)/k_{\mathbf{n}}^2\right)^{-1} + \frac{k_{\mathbf{n}}^4w_0^2}{2\mathsf{D}_r^2}\left[\left(\mathsf{D}_tk_{\mathbf{n}}^2 + w_0^2k_{\mathbf{n}}^2/(2\mathsf{D}_r) + \mathcal{O}(q^4)\right)^{-1}\right.\right. \\ &\quad \left.\left. - \left(\mathsf{D}_tk_{\mathbf{n}}^2 + \mathsf{D}_r + \mathsf{D}_r\mathcal{O}(q^2)\right)^{-1}\right]\right\} + \mathcal{O}(q^4) + \ldots\,,\end{aligned} \tag{46}$$

where $\mathbf{n} = \mathbf{0}$ is explicitly omitted from the sum and the first term in the curly brackets shows the expected $\mathsf{D}_{\mathrm{eff}}^{2\mathrm{D}} = \mathsf{D}_t + w_0^2/(2\mathsf{D}_r)$, equation (29), amended, however, by a correction of order $q^4/k_{\mathbf{n}}^2$. To identify the lowest order correction in $k_{\mathbf{n}}$ and weak potentials, we expand further than equation (45),

$$\lambda_0(q) = -\frac{q^2}{2} + \frac{7q^4}{128} + \mathcal{O}(q^6) = 2w_0^2k_{\mathbf{n}}^2\mathsf{D}_r^{-2} + \frac{7}{8}w_0^4k_{\mathbf{n}}^4\mathsf{D}_r^{-4} + \mathcal{O}(q^6) \tag{47}$$

in the first (of three terms, in the curly bracket) correction term in the sum in equation (46), which gives

$$\rho_0(\mathbf{r}) = L^{-2} - \frac{1}{L^4}\sum_{\mathbf{n}\neq\mathbf{0}}\mathrm{e}^{\imath\mathbf{k}_{\mathbf{n}}\cdot\mathbf{r}}\frac{\Upsilon_{\mathbf{n}}}{\mathsf{D}_{\mathrm{eff}}^{2\mathrm{D}}}\left\{1 + \frac{w_0^2k_{\mathbf{n}}^2}{2\mathsf{D}_r^2}\left(1 - \frac{7}{16}\frac{w_0^2}{\mathsf{D}_r\mathsf{D}_{\mathrm{eff}}^{2\mathrm{D}}}\right) + \mathcal{O}(k_{\mathbf{n}}^4)\right\} + \mathcal{O}(\Upsilon^2) \tag{48}$$

by dropping the last term in equation (46), as it is $\mathcal{O}(k_{\mathbf{n}}^4)$, and not expanding the second term any further, as it is $\mathcal{O}(k_{\mathbf{n}}^2)$ as it stands. The expression above it to be compared to the first order term in the barometric formula, equation (C20), which produces only $-\Upsilon_{\mathbf{n}}/\mathsf{D}_t$ as the first-order summand when setting $\mathbf{w}_0 = \mathbf{0}$. The corrections beyond that, $w_0^2k_{\mathbf{n}}^2(1 - 7/16\ldots)/(2\mathsf{D}_r^2)$, are generically due to the stochastic self-propulsion and amount to more than replacing D_t by $\mathsf{D}_{\mathrm{eff}}^{2\mathrm{D}}$.

While the unity as the first term in the curly brackets of equation (48) reproduces the external potential except for the 0-mode, equation (32*a*), the higher orders in $k_{\mathbf{n}}^2$ and $k_{\mathbf{n}}^4$ correspond to even derivatives, suggesting that a linear potential such as equation (113), does not acquire any corrections, except at a jump due to the imposed periodicity. This, however, is an artefact of equation (48) being an expansion in small $\mathbf{k}_{\mathbf{n}}$.

Equation (48) completes the derivation in the present section. In the next section, we will re-derive MSD $\overline{\mathbf{r}^2}(t)$ and density $\rho_0(\mathbf{r})$ of ABPs in two dimensions at stationarity, in an attempt to recover equations (28) and (46) or (48) in a perturbation theory in small w_0 and small potential.

2.2. Perturbation in small w_0

The starting point of the present derivation is the operator $\mathcal{L}_2$ in equation (5*b*) and the harmonic part of the action equation (11*a*),

$$\mathcal{A}_{02}[\tilde{\chi},\chi] = \int\mathrm{d}^2r\int_0^{2\pi}\mathrm{d}\varphi\int\mathrm{d}t\,\tilde{\chi}(\mathbf{r},\varphi,t)\left(-\partial_t + \mathsf{D}_t\nabla_{\mathbf{r}}^2 + \nabla_\varphi^2 - \mu\right)\chi(\mathbf{r},\varphi,t) \tag{49}$$

which becomes diagonal with

$$\chi(\mathbf{r},\varphi,t) = \int\mathrm{đ}\,\omega\,\mathrm{đ}^2k\sum_{\ell=-\infty}^{\infty}\mathrm{e}^{-\imath\omega t}\mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{r}}\mathrm{e}^{\imath\ell\varphi}\chi_\ell(\mathbf{k},\omega) \tag{50a}$$

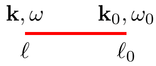
$$\tilde{\chi}(\mathbf{r},\varphi,t) = \int\mathrm{đ}\,\omega\,\mathrm{đ}^2k\sum_{\ell=-\infty}^{\infty}\mathrm{e}^{-\imath\omega t}\mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{r}}\frac{\mathrm{e}^{-\imath\ell\varphi}}{2\pi}\tilde{\chi}_\ell(\mathbf{k},\omega)\ . \tag{50b}$$

Compared to equation (13), in equation (50) the Mathieu functions have been replaced by exponentials,

$$u_\ell\left(\frac{\varphi-\sigma(\mathbf{k})}{2}, q(|\mathbf{k}|)\right) \mapsto \mathrm{e}^{\mathring{\imath}\ell\varphi} \tag{51a}$$

$$\widetilde{u}_\ell\left(\frac{\varphi-\sigma(\mathbf{k})}{2}, q(|\mathbf{k}|)\right) \mapsto \frac{\mathrm{e}^{-\mathring{\imath}\ell\varphi}}{2\pi} \tag{51b}$$

which are orthonormal irrespective of $\mathbf{k}$. The bare propagator of equation (49) can immediately be read off,

$$\langle\chi_\ell(\mathbf{k},\omega)\tilde{\chi}_{\ell_0}(\mathbf{k}_0,\omega_0)\rangle_0 = \frac{\delta_{\ell,\ell_0}\bar{\delta}(\mathbf{k}+\mathbf{k}_0)\bar{\delta}(\omega+\omega_0)}{-\mathring{\imath}\omega+\mathrm{D}_t\mathbf{k}^2+\mathrm{D}_r\ell^2+\mu} = \delta_{\ell,\ell_0}\bar{\delta}(\mathbf{k}+\mathbf{k}_0)\bar{\delta}(\omega+\omega_0)H_\ell(\mathbf{k},\omega) \triangleq$$  $. \quad (52)$

The perturbative part of the action equation (11*b*) includes the self-propulsion, but its precise form depends on whether the system is finite or infinite and thus left to be stated in the sections ahead.

2.2.1. MSD

It is instructive to derive the MSD with harmonic action equation (49), orthogonal system equation (50) and perturbative action equation (11*b*), rewritten as

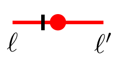
$$\mathcal{A}_{P2} = \int \bar{\mathrm{d}}^2k\,\bar{\mathrm{d}}^2k'\,\bar{\mathrm{d}}\omega \sum_{\ell,\ell'=-\infty}^{\infty} \chi_\ell(\mathbf{k},\omega)\,\tilde{\chi}_{\ell'}(\mathbf{k}',-\omega)\,\frac{w_0}{2}\bar{\delta}(\mathbf{k}+\mathbf{k}')$$
$$\times\left[-\mathring{\imath}k_x(\delta_{\ell',\ell+1}+\delta_{\ell',\ell-1})+k_y(\delta_{\ell',\ell-1}-\delta_{\ell',\ell+1})\right] \tag{53}$$

in the absence of an external potential. To ease notation, we may introduce the coupling

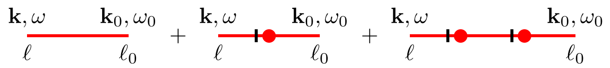
$$W_{\ell',\ell}(\mathbf{k}) = -w_0\int\mathrm{d}\varphi\,\frac{\mathrm{e}^{-\mathring{\imath}\ell'\varphi}}{2\pi}\left(\mathring{\imath}k_x\cos\varphi+\mathring{\imath}k_y\sin\varphi\right)\mathrm{e}^{\mathring{\imath}\ell\varphi} \tag{54a}$$

$$= \frac{w_0}{2}\left[-\mathring{\imath}k_x(\delta_{\ell',\ell+1}+\delta_{\ell',\ell-1})+k_y(\delta_{\ell',\ell-1}-\delta_{\ell',\ell+1})\right] \tag{54b}$$

with $\mathbf{k}=(k_x,k_y)^\intercal$ and $\mathbf{r}=(x,y)^\intercal$. The expression $\mathring{\imath}k_x\cos\varphi+\mathring{\imath}k_y\sin\varphi$ is due to $\mathbf{w}\cdot\nabla_\mathbf{r}$ of the self-propulsion hitting $\mathrm{e}^{\mathring{\imath}\mathbf{kr}}$, equation (2). For the diagrammatics we introduce the self-propulsion vertex

$$W_{\ell',\ell}(\mathbf{k}) \triangleq$$  $, \quad (55)$

so that the full propagator reads

$$\langle\chi_\ell(\mathbf{k},\omega)\tilde{\chi}_{\ell_0}(\mathbf{k}_0,\omega_0)\rangle \triangleq$$  $+\dots$

$$\triangleq \bar{\delta}(\mathbf{k}+\mathbf{k}_0)\bar{\delta}(\omega+\omega_0)\Big(H_\ell(\mathbf{k},\omega)\,\delta_{\ell,\ell_0}+H_\ell(\mathbf{k},\omega)\,W_{\ell,\ell_0}(\mathbf{k})H_{\ell_0}(\mathbf{k},\omega)$$
$$+\sum_{\ell_1}H_\ell(\mathbf{k},\omega)\,W_{\ell,\ell_1}(\mathbf{k})H_{\ell_1}(\mathbf{k},\omega)\,W_{\ell_1,\ell_0}(\mathbf{k})H_{\ell_0}(\mathbf{k},\omega)+\dots\Big) \tag{56}$$

using the notation of equation (52). A marginalisation over φ amounts to evaluating equation (56) at $\ell=0$, equation (50). The MSD can be determined by double differentiation with respect to $\mathbf{k}$ as done in equations (23) and (28). This calculation is simplified by calculating the MSD in x only, i.e. taking $\partial_{k_x}^2$ rather than $\partial_{k_x}^2+\partial_{k_y}^2$. This 'trick', however also requires uniform initialisation in φ_0 to avoid any bias. In summary

$$\overline{\mathbf{r}^2}(t-t_0) = 2\overline{x^2}(t-t_0) = -2\,\partial_{k_x}^2\Big|_{\substack{k_x=0\\k_y=0}}\int_0^{2\pi}\mathrm{d}\varphi\,\frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\varphi_0\int\bar{\mathrm{d}}^2k_0\,\langle\chi(\mathbf{k},\varphi,t)\,\tilde{\chi}(\mathbf{k}_0,\varphi_0,t_0)\rangle \tag{57}$$

where the integral over $\mathbf{k}_0$ is the inverse Fourier transform with $\mathbf{x}_0=\mathbf{0}$ and is trivially taken by using $\bar{\delta}(\mathbf{k}+\mathbf{k}_0)$ due to translational invariance.

The two integrals over φ and φ_0 in equation (57) amount to setting $\ell=0$ and $\ell_0=0$, with all factors of 2π cancelling. Of the three terms in equation (56), the second one, which is the first order correction in the self-propulsion carrying a single factor of the coupling vertex $W_{\ell,\ell_0}(\mathbf{k})$, equation (54*a*), is odd in k_x. Differentiating twice with respect to k_x and evaluating at $k_x=k_y=0$ will thus make it vanish. The third term is quadratic in k_x in the numerator and not singular in k_x in the denominator. The only way for the third term not to vanish at $k_x = k_y = 0$ is when $W_{\ell,\ell_1}(\mathbf{k})W_{\ell_1,\ell_0}(\mathbf{k})$ is differentiated twice with respect to k_x,

$$\partial_{k_x}^2\Big|_{\substack{k_x=0\\k_y=0}} W_{0,\ell_1}(\mathbf{k})W_{\ell_1,0}(\mathbf{k}) = \frac{-w_0^2}{2}\left[\delta_{1,\ell_1}+\delta_{-1,\ell_1}\right] . \tag{58}$$

No higher order terms in w_0 can contribute, as they all carry higher powers of k_x as a pre-factor. We thus arrive at

$$\overline{\mathbf{r}^2}(t-t_0) = \int đ\,\omega\, e^{-\imath\omega(t-t_0)}\left\{\frac{4\mathsf{D}_t}{(-\imath\omega+\mu)^2} + \frac{w_0^2}{(-\imath\omega+\mu)^2}\frac{2}{-\imath\omega+\mathsf{D}_r+\mu}\right\} \tag{59}$$

where the term $2/(-\imath\omega+\mathsf{D}_r+\mu)$ originates from $H_{\ell_1}(\mathbf{k},\omega)$ at $\ell_1=-1,1$ according to equation (58). Taking the inverse Fourier transform from ω to $t-t_0$ then indeed reproduces equation (28) in the limit $\mu\downarrow 0$ with the repeated poles producing the desired factors of $t-t_0$. This confirms that even when the self-propulsion is dealt with perturbatively, observables can be derived in closed form. This is not a triviality, as $w_0^2 t/\mathsf{D}_t$ is a dimensionless quantity and thus might enter to all orders. We proceed in the present framework by allowing for an external potential.

2.2.2. External potential

In this section, we aim to re-derive the density $\rho_0(\mathbf{r})$ of ABPs in an external potential, as initially determined in section 2.1.2. As the self-propulsion is a perturbation, the full perturbative action equations (11*b*) and (53) reads

$$\begin{aligned}\mathcal{A}_{P2} = \int đ\,\omega \frac{1}{L^4}\sum_{\mathbf{n}_1,\mathbf{n}_2}\sum_{\ell_1,\ell_2=-\infty}^{\infty}\chi_{\ell_1}(\mathbf{k}_{\mathbf{n}_1},\omega)\tilde{\chi}_{\ell_2}(\mathbf{k}_{\mathbf{n}_2},-\omega)L^2\delta_{\mathbf{n}_1+\mathbf{n}_2,\mathbf{0}}W_{\ell_2,\ell_1}(\mathbf{k}_{\mathbf{n}_1})\\ +\frac{1}{L^6}\sum_{\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3}L^2\delta_{\mathbf{n}_1+\mathbf{n}_2+\mathbf{n}_3,\mathbf{0}}\sum_{\ell_1,\ell_3}(\mathbf{k}_{\mathbf{n}_1}\cdot\mathbf{k}_{\mathbf{n}_2})\tilde{\chi}_{\ell_1}(\mathbf{k}_{\mathbf{n}_1},-\omega)\Upsilon_{\mathbf{n}_2}\chi_{\ell_3}(\mathbf{k}_{\mathbf{n}_3},\omega)\end{aligned} \tag{60}$$

using the notation $\mathbf{k}_{\mathbf{n}_1} = (k_{n_{1x}},k_{n_{1y}})^\mathsf{T}$. The action equation (60) is based on discrete Fourier modes similar to equation (30) as the system's volume is finite. It deviates from equation (30) but using Fourier modes for the director as in equation (50)

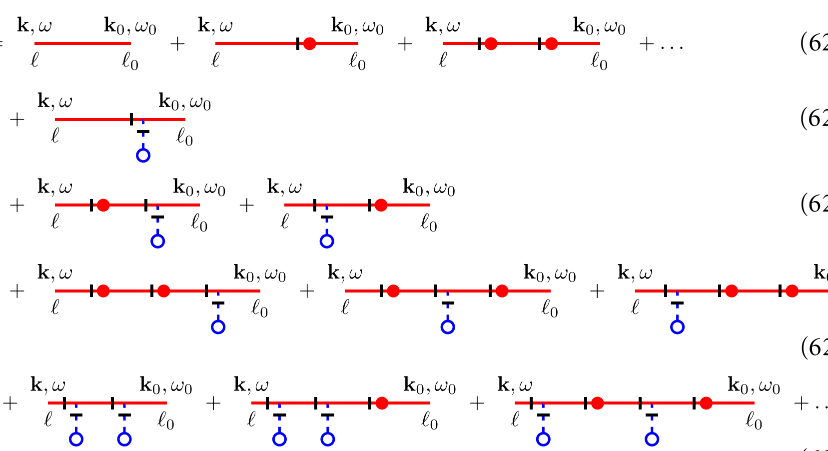
$$\chi(\mathbf{r},\varphi,t) = \int đ\,\omega\frac{1}{L^2}\sum_{\mathbf{n}\in\mathbb{Z}^2}\sum_{\ell=-\infty}^{\infty} e^{-\imath\omega t}e^{\imath\mathbf{k}_\mathbf{n}\cdot\mathbf{r}}e^{\imath\ell\varphi}\chi_\ell(\mathbf{k}_\mathbf{n},\omega) \tag{61a}$$

$$\tilde{\chi}(\mathbf{r},\varphi,t) = \int đ\,\omega\frac{1}{L^2}\sum_{\mathbf{n}\in\mathbb{Z}^2}\sum_{\ell=-\infty}^{\infty} e^{-\imath\omega t}e^{\imath\mathbf{k}_\mathbf{n}\cdot\mathbf{r}}\frac{e^{-\imath\ell\varphi}}{2\pi}\tilde{\chi}_\ell(\mathbf{k}_\mathbf{n},\omega) . \tag{61b}$$

Compared to equation (31*b*), equation (60) has the great benefit of the diagonality of the angular modes in the potential term.

To calculate the particle density $\rho_0(\mathbf{r})$ in the stationary state, equation (36), we expand the full propagator diagrammatically,

$\langle\chi(\mathbf{k},\varphi,\omega)\tilde{\chi}(\mathbf{k}_0,\varphi_0,\omega_0)\rangle =$

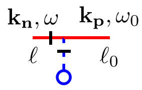


(62*a*) (62*b*) (62*c*) (62*d*) (62*e*)

As in section 2.1.2, taking the limit $t_0 \to -\infty$ amounts to an amputation upon which any diagram vanishes that carries a dashed propagator before (i.e. to the right of) a source of momentum. As a result, only the five leftmost diagrams in equation (62) contribute at stationarity. In the following, we will restrict ourselves to diagrams with at most one bauble, i.e. to first order in the potential. Further, we will incorporate the self-propulsion to second order, leaving us with the four leftmost diagrams in equations (62*a*) and (62*b*).

As seen in section 2.1.2, equation (62*a*) contributes to the density merely with $1/L^2$. The other three diagrams require more detailed attention. Firstly, equation (62*b*) gives

$$D_b(\mathbf{k_n},\ell,\omega;\mathbf{k_p},\ell_0,\omega_0) \triangleq$$



$$\triangleq \delta_{\ell,\ell_0}\delta(\omega+\omega_0)H_\ell(\mathbf{k_n},\omega)(-\mathbf{k_n}\cdot\mathbf{k_{n+p}})\Upsilon_{\mathbf{n+p}}H_{\ell_0}(-\mathbf{k_p},\omega)\ , \tag{63}$$

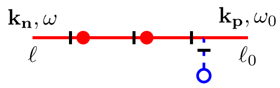
using equation (52) for $H_\ell(\mathbf{k_n},\omega)$. Upon taking the inverse Fourier transform in ω and ω_0, the limit $t_0 \to -\infty$ can be taken, replacing the incoming leg $H_{\ell_0}(\mathbf{k_p},\omega_0)$ effectively by $\delta_{\mathbf{p},\mathbf{0}}\delta_{\ell_0,0}$. After transforming from ℓ,ℓ_0 to φ,φ_0 and taking the integral over φ all factors of 2π have cancelled, leaving of equation (63)

$$\lim_{t_0\to-\infty}\int_0^{2\pi}\mathrm{d}\varphi\, D_b(\mathbf{r},\varphi,t;\mathbf{r}_0,\varphi_0,t_0) = \frac{1}{L^4}\sum_{\mathbf{n}}\mathrm{e}^{\mathring{\imath}\mathbf{k_n}\cdot\mathbf{r}}H_0(\mathbf{k_n},0)(-\mathbf{k_n}\cdot\mathbf{k_n})\Upsilon_{\mathbf{n}} \overset{\mu\downarrow 0}{=} -\frac{1}{L^4}\sum_{\mathbf{n}\neq\mathbf{0}}\mathrm{e}^{\mathring{\imath}\mathbf{k_n}\cdot\mathbf{r}}\frac{\Upsilon_{\mathbf{n}}}{\mathsf{D}_t} \tag{64}$$

as $H_0(\mathbf{k_n},0) = (\mathsf{D}_t k_{\mathbf{n}}^2+\mu)^{-1}$, whose factor $k_{\mathbf{n}}^{-2}$ cancels with $\mathbf{k_n}\cdot\mathbf{k_n}$ unless $\mathbf{k_n}=\mathbf{0}$, in which case the expression vanishes. Equation (64) is the lowest order correction in both Υ and w_0 to the density.

Of the remaining two diagrams, the leftmost in equations (62*c*) and (62*d*), only the latter contributes once $t_0\to-\infty$ forces $\ell_0=0$ and $\int\mathrm{d}\varphi$ forces $\ell=0$, because the single coupling vertex, equation (54*a*), requires the angular modes to be offset by 1. The only diagram left to consider is thus

$$D_d(\mathbf{k_n},\ell,\omega;\mathbf{k_p},\ell_0,\omega_0) \triangleq$$



$$\triangleq H_\ell(\mathbf{k_n},\omega)\left(\sum_{\ell_1}W_{\ell,\ell_1}(\mathbf{k_n})H_{\ell_1}(\mathbf{k_n},\omega)W_{\ell_1,\ell_0}(\mathbf{k_n})\right)H_{\ell_0}(\mathbf{k_n},\omega)(-\mathbf{k_n}\cdot\mathbf{k_{n+p}})\Upsilon_{\mathbf{n+p}}H_{\ell_0}(-\mathbf{k_p},\omega)\delta(\omega+\omega_0)\ . \tag{65}$$

After taking $t_0\to-\infty$ and $\int\mathrm{d}\varphi$, the only two contributions from the sum are $\ell_1=-1,1$, so that

$$\lim_{t_0\to-\infty}\int_0^{2\pi}\mathrm{d}\varphi\, D_d(\mathbf{r},\varphi,t;\mathbf{r}_0,\varphi_0,t_0) = \frac{1}{2L^4}\sum_{\mathbf{n}}\mathrm{e}^{\mathring{\imath}\mathbf{k_n}\cdot\mathbf{r}}w_0^2k_{\mathbf{n}}^4\Upsilon_{\mathbf{n}}\left(\mathsf{D}_t k_{\mathbf{n}}^2+\mu\right)^{-2}\left(\mathsf{D}_t k_{\mathbf{n}}^2+\mathsf{D}_r+\mu\right)^{-1} \tag{66}$$

using

$$W_{0,\pm1}(\mathbf{k}) = -\frac{w_0}{2}\left[\mathring{\imath}k_x\pm k_y\right] \quad\text{and}\quad W_{\pm1,0}(\mathbf{k}) = \frac{w_0}{2}\left[-\mathring{\imath}k_x\pm k_y\right] \tag{67}$$

from equation (54*a*), so that $W_{0,1}(\mathbf{k})W_{1,0}(\mathbf{k}) = W_{0,-1}(\mathbf{k})W_{-1,0}(\mathbf{k}) = -w_0^2k^2/4$. After taking the limit $\mu\downarrow 0$ in equation (66) the factor $k_{\mathbf{n}}^4$ cancels with the same factor in $(\mathsf{D}_t k_{\mathbf{n}}^2+\mu)^{-2}$ whenever $\mathbf{n}\neq\mathbf{0}$, so that finally

$$\rho_0(\mathbf{r}) = L^{-2} + \lim_{\mu\downarrow 0}\lim_{t_0\to-\infty}\int_0^{2\pi}\mathrm{d}\varphi\, D_b(\mathbf{r},\varphi,t;\mathbf{r}_0,\varphi_0,t_0) + D_d(\mathbf{r},\varphi,t;\mathbf{r}_0,\varphi_0,t_0) \tag{68a}$$

$$= L^{-2} - \frac{1}{L^4}\sum_{\mathbf{n}\neq\mathbf{0}}\mathrm{e}^{\mathring{\imath}\mathbf{k_n}\cdot\mathbf{r}}\frac{\Upsilon_{\mathbf{n}}}{\mathsf{D}_t}\left\{1-\frac{w_0^2}{2\mathsf{D}_t}\left(\mathsf{D}_t k_{\mathbf{n}}^2+\mathsf{D}_r\right)^{-1}\right\} + \mathcal{O}\left(w_0^4\right) + \dots \tag{68b}$$

to be compared to the purely drift-diffusive equation (C20) and to equations (46) or (48), derived using Mathieu functions, rather than the perturbative approach to self-propulsion here. By inspection of the two expressions, equations (46) and (68*b*), the two are equivalent provided

$$1-\frac{w_0^2}{2\mathsf{D}_t}\left(\mathsf{D}_t k_{\mathbf{n}}^2+\mathsf{D}_r\right)^{-1}+\mathcal{O}\left(w_0^4\right) = \mathsf{D}_t\left\{\left(\mathsf{D}_t+w_0^2/(2\mathsf{D}_r)+\mathcal{O}\left(q^4\right)/k_{\mathbf{n}}^2\right)^{-1} + \frac{k_{\mathbf{n}}^4w_0^2}{2\mathsf{D}_r^2}\left[\left(\mathsf{D}_t k_{\mathbf{n}}^2+w_0^2k_{\mathbf{n}}^2/(2\mathsf{D}_r)+\mathcal{O}\left(q^4\right)\right)^{-1}-\left(\mathsf{D}_t k_{\mathbf{n}}^2+\mathsf{D}_r+\mathsf{D}_r\mathcal{O}\left(q^2\right)\right)^{-1}\right]\right\} \tag{69}$$

which can indeed be shown by expanding all terms on the right hand side to order w_0^2 only, absorbing all other terms into $\mathcal{O}(w_0^4)$, for example

$$\mathsf{D}_t\left(\mathsf{D}_t + w_0^2/\left(2\mathsf{D}_r\right) + \mathcal{O}\left(q^4\right)/k_{\mathbf{n}}^2\right)^{-1} = 1 - \frac{w_0^2}{2\mathsf{D}_t\mathsf{D}_r} + \mathcal{O}\left(w_0^4\right) \ . \tag{70}$$

The term generically due to the activity in equation (68*b*) is $w_0^2/(2\mathsf{D}_t(\mathsf{D}_t k_{\mathbf{n}}^2 + \mathsf{D}_r))$, by comparison to equation (C20).

This concludes the discussion of ABPs in two dimensions. In the following sections, we will calculate MSD and density in an external potential for ABPs in three dimensions, using the above as a template.

3. ABPs in three dimensions

In three spatial dimensions, the diffusion of the director takes place on a curved manifold, which renders the Laplacian rather unwieldy, equation (3). The spherical harmonics provide a suitable eigensystem for this operator, but the self-propulsion term spoils the diagonalisation. As in the two-dimensional case, section 2, there are two possible ways ahead: Either find suitable special functions or deal with the self-propulsion term perturbatively. In the following subsection, we focus on the former, in section 3.2 on the latter.

3.1. 'Three-dimensional Mathieu functions'

The harmonic part of the action is equation (9) with equations (2) and (3) in equation (5*a*), more explicitly

$$\begin{aligned}\mathcal{A}_{01}[\tilde{\chi},\chi] = \int \mathrm{d}^3x \int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi \sin\theta \int \mathrm{d}t\, \tilde{\chi}(\mathbf{r},\theta,\varphi,t)\Big(-\partial_t + \mathsf{D}_t\nabla_{\mathbf{r}}^2 - w_0\left(\sin\theta\cos\varphi\,\partial_x + \sin\theta\sin\varphi\,\partial_y + \cos\theta\,\partial_z\right)\\ + \mathsf{D}_r\left(\frac{1}{\sin\theta}\partial_\theta\sin\theta\,\partial_\theta + \frac{1}{\sin^2\theta}\partial_\varphi^2\right) - \mu\Big)\chi(\mathbf{r},\theta,\varphi,t)\end{aligned} \tag{71}$$

using the notation $\mathbf{r} = (x,y,z)^\mathsf{T}$.

The eigensystem that we will use now is modelled along the two-dimensional Mathieu functions, equation (13). Specifically, it is

$$\chi(\mathbf{r},\theta,\varphi,t) = \int đ\omega đ^3k \sum_{\ell=0}^{\infty}\sum_m \mathrm{e}^{-\imath\omega t}\mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{r}} u_\ell^m\left(\theta - \tau(\mathbf{k}), \varphi - \sigma(\mathbf{k}), \mathbf{q}(\mathbf{k})\right)\chi_\ell^m(\mathbf{k},\omega) \tag{72a}$$

$$\tilde{\chi}(\mathbf{r},\theta,\varphi,t) = \int đ\omega đ^3k \sum_{\ell=0}^{\infty}\sum_m \mathrm{e}^{-\imath\omega t}\mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{r}} \tilde{u}_\ell^m\left(\theta - \tau(-\mathbf{k}), \varphi - \sigma(-\mathbf{k}), \mathbf{q}(-\mathbf{k})\right)\tilde{\chi}_\ell^m(\mathbf{k},\omega) \tag{72b}$$

with

$$\tilde{u}_\ell^m(\theta,\varphi,\mathbf{q}(\mathbf{k})) = \frac{1}{4\pi}u_\ell^m(\theta,\varphi,\mathbf{q}(\mathbf{k})) \tag{73}$$

defined as eigenfunctions via equation (76), similar to equation (19). These functions are orthonormal, similar to equation (15),

$$\begin{aligned}&\delta\!\!\!^{-}(\mathbf{k}+\mathbf{k}')\int_0^\pi \mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\varphi\sin\theta\, u_\ell^m\left(\theta-\tau(\mathbf{k}),\varphi-\sigma(\mathbf{k}),\mathbf{q}(\mathbf{k})\right)\tilde{u}_{\ell'}^{m'}\left(\theta-\tau(-\mathbf{k}),\varphi-\sigma(-\mathbf{k}),\mathbf{q}(-\mathbf{k}')\right)\\&= \delta\!\!\!^{-}(\mathbf{k}+\mathbf{k}')\,\delta_{\ell,\ell'}\delta_{m,m'}\end{aligned} \tag{74}$$

with $q(|\mathbf{k}|)$ of the two-dimensional case, equation (14), replaced by

$$\mathbf{q}(\mathbf{k}) = \imath\frac{w_0\mathbf{k}}{\mathsf{D}_r} \tag{75}$$

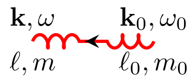
and two instead of one arbitrary functions $\sigma(\mathbf{k})$ and $\tau(\mathbf{k})$, *cf* equation (15). The benefit of those, however, is rather limited compared to the two-dimensional case, where $\mathbf{k}\cdot\mathbf{w}$ was rewritten as $kw_0\cos(\varphi-\alpha)$. We therefore choose $\sigma\equiv\tau\equiv 0$ and demand

$$\left(-\mathring{\imath}\frac{w_0}{\mathsf{D}_r}\left(k_x\sin\theta\cos\varphi+k_y\sin\theta\sin\varphi+k_z\cos\theta\right)+\frac{1}{\sin\theta}\partial_\theta\sin\theta\partial_\theta+\frac{1}{\sin^2\theta}\partial_\varphi^2\right)u_\ell^m(\theta,\varphi,\mathbf{q})$$
$$=-\lambda_\ell^m(\mathbf{q})\,u_\ell^m(\theta,\varphi,\mathbf{q})\ . \tag{76}$$

These eigenfunctions are characterised in some detail in appendix A. For now, it suffices to know that they exist and that the eigenvalues $\lambda_\ell^m(\mathbf{q})$ are indeed discrete and indexed in both ℓ and m. Having relegated the details of the eigensystem to the appendix, the bare propagator can now be determined without much ado,

$$\left\langle\chi_\ell^m(\mathbf{k},\omega)\,\tilde{\chi}_{\ell_0}^{m_0}(\mathbf{k}_0,\omega_0)\right\rangle_0=\frac{\delta_{\ell,\ell_0}\delta_{m,m_0}\bar{\delta}\left(\mathbf{k}+\mathbf{k}_0\right)\bar{\delta}\left(\omega+\omega_0\right)}{-\mathring{\imath}\omega+\mathsf{D}_t\mathbf{k}^2+\mathsf{D}_r\lambda_\ell^m\left(\mathbf{q}\left(\mathbf{k}\right)\right)+\mu}=\delta_{\ell,\ell_0}\delta_{m,m_0}\bar{\delta}\left(\mathbf{k}+\mathbf{k}_0\right)\bar{\delta}\left(\omega+\omega_0\right)G_\ell^m\left(\mathbf{k},\omega\right) \tag{77a}$$

$$\triangleq \tag{77b}$$



and we proceed with the MSD.

3.1.1. MSD

The MSD derives from the propagator equation (77*a*) via a double derivative. As in the two-dimensional case, the derivation simplifies considerably with uniform initialisation. Further, because the eigenequation (76) is particularly simple whenever $k_x=k_y=0$, we may write the MSD in terms of derivatives with respect to k_z only,

$$\overline{\mathbf{r}^2}(t)=-3\,\partial_{k_z}^2\big|_{\mathbf{k}=\mathbf{0}}\int_0^\pi\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\varphi\,\sin\theta\,\frac{1}{4\pi}\int_0^\pi\mathrm{d}\theta_0\int_0^{2\pi}\mathrm{d}\varphi_0\,\sin\theta_0$$
$$\times\sum_{\ell=0}^{\infty}\sum_m u_\ell^m\left(\theta,\varphi,\mathbf{q}\left(k_z\mathbf{e}_z\right)\right)\tilde{u}_{\ell'}^{m'}\left(\varphi_0,\theta_0,\mathbf{q}\left(k_z\mathbf{e}_z\right)\right)\mathrm{e}^{-\left(\mathsf{D}_tk^2+\mathsf{D}_r\lambda_\ell^m\left(\mathbf{q}\left(k_z\mathbf{e}_z\right)\right)\right)t}. \tag{78}$$

Similar to equation (24), we use coefficients

$$\int_0^\pi\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\varphi\,\sin\theta\,u_\ell^m(\theta,\varphi,\mathbf{q}(k_z\mathbf{e}_z)))=4\pi\,A_{\ell,0}^{0,0}(q\mathbf{e}_z)\delta_{m,0} \tag{79}$$

as derived in more detail in equation (A27). These coefficients we need to determine at most up to order q^2 in order to express $\overline{\mathbf{r}^2}(t)$ in closed form. Using the notation $q=\mathring{\imath}w_0k_z/\mathsf{D}_r$ in $\mathbf{q}(k_z\mathbf{e}_z)=q\mathbf{e}_z$, equation (78) produces with equation (79)

$$\overline{\mathbf{r}^2}(t)=-3\,\partial_{k_z}^2\big|_{\mathbf{k}=\mathbf{0}}\left\{\left(1-\frac{q^2}{24}\right)^2\mathrm{e}^{-(\mathsf{D}_tk_z^2+\mathsf{D}_r\lambda_0^0(q\mathbf{e}_z)t)}+\left(\frac{q}{2\sqrt{3}}\right)^2\mathrm{e}^{-(\mathsf{D}_tk_z^2+\mathsf{D}_r\lambda_1^0(q\mathbf{e}_z)}\right\} \tag{80}$$

from the expansion of $A_{0,0}^{0,0}(q\mathbf{e}_z)$, equation (A22*a*), and $A_{1,0}^{0,0}(q\mathbf{e}_z)$, equation (A23*a*), with $A_{\ell,0}^{0,0}(q\mathbf{e}_z)\in\mathcal{O}\left(q^2\right)$ for $\ell\geqslant 2$, equation (A24). The two eigenvalues $\lambda_0^0(q\mathbf{e}_z)=-q^2/6+\ldots$ and $\lambda_1^0(q\mathbf{e}_z)=2+\ldots$, equations (A18) and (A20), need to be known only to leading order in q. Performing the derivative and re-arranging terms then produces the final result

$$\overline{\mathbf{r}^2}(t)=6\mathsf{D}_tt+\frac{w_0^2}{2\mathsf{D}_r^2}\left(\mathrm{e}^{-2\mathsf{D}_rt}-1+2\mathsf{D}_rt\right) \tag{81}$$

structurally similar to the result in two dimensions, equation (28), and indeed identical to the MSD of RnT particles in three dimensions, equation (49) of [11], if the tumble rate α is replaced by $2\mathsf{D}_r$ [3, 4]. The effective diffusion constant in three dimensions [39] is

$$\mathsf{D}_{\mathrm{eff}}^{3\mathrm{D}}=\mathsf{D}_t+\frac{w_0^2}{6\mathsf{D}_r}\ , \tag{82}$$

to be compared to equation (29).

3.1.2. External potential

Allowing for an external potential and confining the particles to a finite space means that the fields are now written as

$$\chi(\mathbf{r},\theta,\varphi,t) = \int đ\,\omega \frac{1}{L^3} \sum_{\mathbf{n}\in\mathbb{Z}^3} \sum_{\ell=0}^{\infty} \sum_{m} \mathrm{e}^{-\imath\omega t} \mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{r}} u_\ell^m(\theta,\varphi,\mathbf{q}(\mathbf{k}))\,\chi_\ell(\mathbf{k},\omega) \tag{83a}$$

$$\tilde{\chi}(\mathbf{r},\theta,\varphi,t) = \int đ\,\omega \frac{1}{L^3} \sum_{\mathbf{n}\in\mathbb{Z}^3} \sum_{\ell=0}^{\infty} \sum_{m} \mathrm{e}^{-\imath\omega t} \mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{r}} \tilde{u}_{\ell'}^{m'}(\theta,\varphi,\mathbf{q}(-\mathbf{k}))\,\tilde{\chi}_\ell(\mathbf{k},\omega) \tag{83b}$$

similar to equations (30) and (72) and any expectation needs to be taken with the perturbative action

$$\mathcal{A}_{P1} = \int đ\,\omega \frac{1}{L^9} \sum_{\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3} L^3 \delta_{\mathbf{n}_1+\mathbf{n}_2+\mathbf{n}_3,\mathbf{0}} \sum_{\ell_1,\ell_3} \sum_{m_1,m_3} (\mathbf{k}_{\mathbf{n}_1}\cdot\mathbf{k}_{\mathbf{n}_2})\,\tilde{\chi}_{\ell_1,m_1}(\mathbf{k}_{\mathbf{n}_1},-\omega)\,\Upsilon_{\mathbf{n}_2}\chi_{\ell_3,m_3}(\mathbf{k}_{\mathbf{n}_3},\omega)\,\Delta_{\ell_1,\ell_3}^{m_1,m_3}(-\mathbf{k}_{\mathbf{n}_1},-\mathbf{k}_{\mathbf{n}_3}) \,, \tag{84}$$

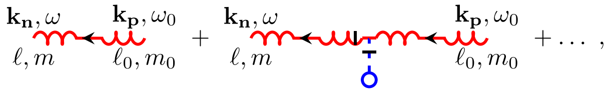
similar to equation (34) with integral

$$\Delta_{\ell_1,\ell_3}^{m_1,m_3}(-\mathbf{k}_{\mathbf{n}_1},-\mathbf{k}_{\mathbf{n}_3}) = \int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi\, \sin\theta\, u_{\ell_3}^{m_3}(\theta,\varphi\mathbf{q}(\mathbf{k}_{\mathbf{n}_3}))\,\tilde{u}_{\ell_1}^{m_1}(\theta,\varphi\mathbf{q}(\mathbf{k}_{\mathbf{n}_1}))\,, \tag{85}$$

similar to equation (33).

The resulting diagrammatics of the full propagator to leading order in the potential is

$$\langle\chi(\mathbf{k_n},\ell,m,\omega)\tilde{\chi}(\mathbf{k_p},\ell_0,m_0,\omega_0)\rangle \triangleq \tag{86}$$



as in equation (37) but with the index ℓ replaced by the couple ℓ,m. The arguments that follow to extract the stationary density are similar to those in section 2.1.2. Yet, to be able to draw on the results in appendix A, all $\mathbf{k}$-vectors featuring in the three-dimensional Mathieu functions need to be parallel to $\mathbf{e}_z$. Because amputated diagrams draw all $\mathbf{k}$-dependence from spatial variation of the potential, we thus demand $\Upsilon(\mathbf{r}) = \Upsilon(z)$, i.e. that the potential depends only on the z-component of $\mathbf{r} = (x,y,z)^\mathsf{T}$. Its Fourier transform can therefore be written in the form

$$\Upsilon_\mathbf{n} = \iiint_0^L \mathrm{d}^3r\,\Upsilon(\mathbf{r})\,\mathrm{e}^{-\imath\mathbf{k_n}\cdot\mathbf{r}} = L^2\delta_{n_x,0}\delta_{n_y,0}\Upsilon_{n_z} \tag{87}$$

where $\mathbf{n} = (n_x,n_y,n_z)^\mathsf{T}$. The notation of equation (87) is slightly ambiguous, as Υ_{n_z} on the right is a Fourier transform in the z-direction only, while $\Upsilon_\mathbf{n}$ on the left is a Fourier transform in all space, yet the alternatives seem to obfuscate even more.

Just like in section 2.1.2, the stationary limit enforces $\mathbf{k_p} = \mathbf{0}$, as well as $\ell_0 = 0$, as otherwise $\lambda_\ell^m(\mathbf{q}(0)) \neq 0$, equation (A5*b*), in the propagator equation (77*a*).

Turning our attention to the projection $\Delta_{\ell_1,0}^{m_1,m_3}(\mathbf{k_n},\mathbf{k_p})$ for $\mathbf{p}=\mathbf{0}$, this vanishes whenever $m_3 \neq 0$ as $u_{\ell=0}^m(\theta,\varphi,\mathbf{q}=\mathbf{0}) = \sqrt{4\pi}Y_0^m(\theta,\varphi) = \delta_{m,0}$, equation (A6), because the spherical harmonics that the three-dimensional Mathieu functions are written in with $\ell=0$ allow only for $m=0$, so that $Y_0^m(\theta,\varphi) = \delta_{m,0}/\sqrt{4\pi}$. It follows that

$$\Delta_{\ell,0}^{m,m_0}(\mathbf{k_n},\mathbf{0}) = \delta_{m_0,0}\int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi\,\sin\theta\, u_\ell^m(\theta,\varphi,\mathbf{q}(\mathbf{k_n})) = \delta_{m_0,0}\delta_{m,0}A_{\ell,0}^{0,0}(\mathbf{q}(\mathbf{k_n}))\,, \tag{88}$$

for all $\mathbf{k_n} \parallel \mathbf{e}_z$. Equation (88) corresponds to equation (41). This produces

$$\begin{aligned}\lim_{t_0\to-\infty}\left\langle\chi(\mathbf{k_n},\theta,\varphi,t)\,\tilde{\chi}\left(\mathbf{k_p},\theta_0,\varphi_0,t_0\right)\right\rangle &= u_0^0(\theta,\varphi,\mathbf{0})\,\tilde{u}_0^0(\theta_0,\varphi_0,\mathbf{0})\,L^2\delta_{\mathbf{n+p},\mathbf{0}}\delta_{\mathbf{p},\mathbf{0}}\\ &+\sum_{\ell=0}^\infty\sum_m(-\mathbf{k_n}\cdot\mathbf{k_{n+p}})\,\Upsilon_{\mathbf{n+p}}G_\ell^m(\mathbf{k_n},0)\,\delta_{\mathbf{p},\mathbf{0}}\delta_{m,0}A_{\ell,0}^{0,0}(\mathbf{q}(\mathbf{k_n}))\,u_\ell^m(\theta,\varphi,\mathbf{q}(\mathbf{k_n}))\,\tilde{u}_0^0(\theta_0,\varphi_0,\mathbf{0})+\dots\,.\end{aligned} \tag{89}$$

similar to equation (42), with $G_\ell^m(\mathbf{k_n},0)$ denoting the bare propagator equation (77a) and again assuming $\mathbf{k_n} \parallel \mathbf{e}_z$. This is guaranteed by equation (87), which means that $\Upsilon_\mathbf{n}$ vanishes for all $\mathbf{k_n} \nparallel \mathbf{e}_z$, so that the second term in equation (89) only ever contributes when $\mathbf{k_n} \parallel \mathbf{e}_z$.

Since $\widetilde{u}_0^0(\theta_0,\varphi_0,\mathbf{0}) = 1/(4\pi)$, it cancels the 4π of the integral over the final angles θ and φ of both terms on the right hand side of equation (89), the second one by equation (79),

$$\int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi \sin\theta \lim_{t_0\to-\infty} \left\langle \chi(\mathbf{k_n},\theta,\varphi,t)\,\tilde{\chi}(\mathbf{k_p},\theta_0,\varphi_0,t_0)\right\rangle$$
$$= L^3\delta_{\mathbf{n+p},\mathbf{0}}\delta_{\mathbf{p},\mathbf{0}} + \sum_{\ell=0}^{\infty}\left(-\mathbf{k_n}\cdot\mathbf{k_{n+p}}\right)\Upsilon_{\mathbf{n+p}}G_\ell^m(\mathbf{k_n},0)\,\delta_{\mathbf{p},\mathbf{0}}\delta_{m,0}\left(A_{\ell,0}^{0,0}(\mathbf{q}(\mathbf{k_n}))\right)^2 + \dots, \tag{90}$$

similar to equation (43). Expanding to order $q^2 = -w_0^2k_z^2/\mathsf{D}_r^2$, equation (75), means to keep only $\ell = 0, 1$ in the sum in equation (90), as $A_{\ell,0}^{0,0}(q\mathbf{e}_z) \in \mathcal{O}(q^\ell)$, equation (A24). This produces an expression similar to equation (44), and using equations (A22a) and (A23a) for $A_{\ell,0}^{0,0}$, as well as equations (A18) and (A20) for λ_ℓ^0, finally gives

$$\rho_0(\mathbf{r}) = L^{-3} - \frac{1}{L^4}\sum_{n_z\neq0} \mathrm{e}^{\mathring{\imath}zk_{n_z}}\Upsilon_{n_z}\left\{\left(\mathsf{D}_t + w_0^2/(6\mathsf{D}_r) + \mathcal{O}\left(q^4\right)/k_{n_z}^2\right)^{-1} + \frac{k_{n_z}^4w_0^2}{12\mathsf{D}_r^2}\left[\left(\mathsf{D}_tk_{n_z}^2 + w_0^2k_{n_z}^2/(6\mathsf{D}_r) + \mathcal{O}\left(q^4\right)\right)^{-1}\right.\right.$$
$$\left.\left. - \left(\mathsf{D}_tk_{n_z}^2 + 2\mathsf{D}_r + \mathsf{D}_r\mathcal{O}\left(q^2\right)\right)^{-1}\right]\right\} + \mathcal{O}\left(q^4\right) + \dots, \tag{91}$$

using $\mathbf{r} = (x,y,z)^\mathsf{T}$ for the position, $k_{n_z} = 2\pi n_z/L$ for the mode, and equation (87), which cancels L^2. Equation (91) corresponds to equation (46) in two dimension. Expanding rather in small k_{n_z}, similar to equation (48), produces

$$\rho_0(\mathbf{r}) = L^{-3} - \frac{1}{L^4}\sum_{n_z\neq0}\mathrm{e}^{\mathring{\imath}zk_{n_z}}\frac{\Upsilon_{n_z}}{\mathsf{D}_{\mathrm{eff}}^{3\mathrm{D}}}\left\{1 + \frac{w_0^2k_{n_z}^2}{12\mathsf{D}_r^2}\left(1 - \frac{11}{90}\frac{w_0^2}{\mathsf{D}_r\mathsf{D}_{\mathrm{eff}}^{3\mathrm{D}}}\right) + \mathcal{O}\left(k_\mathbf{n}^4\right)\right\} + \mathcal{O}\left(\Upsilon^2\right) \tag{92}$$

which has non-trivial corrections in the form $w_0^2k_{n_z}^2/(12\mathsf{D}_r^2)(\dots)$, compared to the purely drift-diffusive equation (C20), beyond setting in the latter $\mathbf{w}_0 = \mathbf{0}$ and replacing the diffusion constant D_t by $\mathsf{D}_{\mathrm{eff}}^{3\mathrm{D}}$ of equation (82). The difference in L^{-4} compared to L^{-2d} in equation (C20) is solely due to the definition of Υ_{n_z} in equation (87).

This concludes the calculation of properties of three-dimensional ABPs on the basis of 'three-dimensional Mathieu functions'. In the next two sections, we will reproduce the results above on the basis of a perturbation theory in the drift.

3.2. Perturbation in small w_0

Along the lines of section 2.2, we return now to calculate the MSD and the stationary density while treating the self-propulsion as a perturbation over diffusion, so that we can use the eigensystem

$$\chi(\mathbf{r},\theta,\varphi,t) = \int \mathrm{đ}\,\omega\mathrm{đ}^3k\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\mathrm{e}^{-\mathring{\imath}\omega t}\mathrm{e}^{\mathring{\imath}\mathbf{k}\cdot\mathbf{r}}(4\pi)^{1/2}\,Y_\ell^m(\theta,\varphi)\,\chi_\ell^m(\mathbf{k},\omega) \tag{93a}$$

$$\tilde{\chi}(\mathbf{r},\theta,\varphi,t) = \int \mathrm{đ}\,\omega\mathrm{đ}^3k\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\mathrm{e}^{-\mathring{\imath}\omega t}\mathrm{e}^{\mathring{\imath}\mathbf{k}\cdot\mathbf{r}}(4\pi)^{-1/2}\left(Y_\ell^m(\theta,\varphi)\right)^*\tilde{\chi}_\ell^m(\mathbf{k},\omega)\ . \tag{93b}$$

where

$$Y_\ell^m(\theta,\varphi) = \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}P_\ell^m(\cos\theta)\,\mathrm{e}^{\mathring{\imath}m\varphi} \tag{94}$$

denote the well-known spherical harmonics with P_ℓ^m denoting the standard associated Legendre polynomials which carry a factor $(-1)^m$ in their definition, so that, for example $Y_1^1(\theta,\varphi) = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\mathrm{e}^{\mathring{\imath}\varphi}$. Our definition of Y_ℓ^m conforms to `SphericalHarmonicsY[`ℓ, m, θ, φ`]` [41]. The spherical harmonics Y_ℓ^m are orthonormal

$$\int_0^\pi \mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\varphi\sin\theta\,Y_\ell^m(\theta,\varphi)\left(Y_{\ell'}^{m'}(\theta,\varphi)\right)^* = \delta_{\ell,\ell'}\delta_{m,m'} \tag{95}$$

and obey the eigenvalue equation

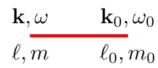
$$\nabla_\Omega^2 Y_\ell^m(\theta,\varphi) = \left(\frac{1}{\sin\theta}\partial_\theta \sin\theta\, \partial_\theta + \frac{1}{\sin^2\theta}\partial_\varphi^2\right) Y_\ell^m(\theta,\varphi) = -\ell(\ell+1)\, Y_\ell^m(\theta,\varphi)\ . \tag{96}$$

The harmonic part of the action equation (11a) now reads

$$\mathcal{A}_{02}[\tilde{\chi},\chi] = -\int \mathrm{d}\omega \,\text{đ}^3 k \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} \tilde{\chi}_\ell^m(-\mathbf{k},-\omega)\left(-\mathring{\imath}\omega + \mathsf{D}_t k^2 + \mathsf{D}_r \ell(\ell+1) + \mu\right)\chi_\ell^m(\mathbf{k},\omega) \tag{97}$$

so that the bare propagators are

$$\left\langle \chi_\ell^m(\mathbf{k},\omega)\tilde{\chi}_{\ell_0}^{m_0}(\mathbf{k}_0,\omega_0)\right\rangle_0 = \frac{\delta_{\ell,\ell_0}\delta_{m,m_0}\text{đ}(\mathbf{k}+\mathbf{k}_0)\text{đ}(\omega+\omega_0)}{-\mathring{\imath}\omega + \mathsf{D}_t\mathbf{k}^2 + \mathsf{D}_r\ell(\ell+1) + m} = \delta_{\ell,\ell_0}\delta_{m,m_0}\text{đ}(\mathbf{k}+\mathbf{k}_0)\text{đ}(\omega+\omega_0) H_\ell^m(\mathbf{k},\omega) \triangleq \tag{98}$$



differing from equation (52) only by the additional factor δ_{m,m_0} and by the eigenvalue of the spherical Laplacian being $\ell(\ell+1)$ rather than ℓ^2. In the absence of an external potential the perturbative part of the action reads

$$\mathcal{A}_{P2} = \int \text{đ}^3 k \mathrm{d}^3 k' \text{đ}\,\omega \sum_{\ell,\ell'=0}^{\infty}\sum_{m=-\ell}^{\ell}\sum_{m'=-\ell'}^{\ell'} \chi_\ell^m(\mathbf{k},\omega)\,\tilde{\chi}_{\ell'}^{m'}(\mathbf{k}',-\omega)\,\text{đ}\,(\mathbf{k}+\mathbf{k}')\,W_{\ell',\ell}^{m',m}(\mathbf{k}) \tag{99}$$

similar to equation (53) with coupling vertex

$$W_{\ell',\ell}^{m',m}(\mathbf{k}) = -w_0\int_0^\pi \mathrm{d}\theta \int_0^{2\pi}\mathrm{d}\varphi\,\sin\theta\left(Y_{\ell'}^{m'}(\theta,\varphi)\right)^*\left(\mathring{\imath}k_x\sin\theta\cos\varphi + \mathring{\imath}k_y\sin\theta\sin\varphi + \mathring{\imath}k_z\cos\theta\right)Y_\ell^m(\theta,\varphi)\,. \tag{100}$$

In principle, any product like $\sin\theta\cos\varphi\, Y_\ell^m(\theta,\varphi)$ can be written in terms of a sum of spherical harmonics (see appendix B),

$$\sin\theta\cos\varphi\, Y_\ell^m(\theta,\varphi) = \sum_{L,M}\sqrt{\frac{2\ell+1}{2(2L+1)}}\,c_{1,0,\ell,0}^{L,0}\, Y_L^M(\theta,\varphi)\left(-c_{1,1,\ell,m}^{L,M} + c_{1,-1,\ell,m}^{L,M}\right)\ , \tag{101a}$$

$$\sin\theta\sin\varphi\, Y_\ell^m(\theta,\varphi) = \mathring{\imath}\sum_{L,M}\sqrt{\frac{2\ell+1}{2(2L+1)}}\,c_{1,0,\ell,0}^{L,0}\, Y_L^M(\theta,\varphi)\left(c_{1,1,\ell,m}^{L,M} + c_{1,-1,\ell,m}^{L,M}\right)\ , \tag{101b}$$

$$\cos\theta Y_\ell^m(\theta,\varphi) = \sum_{L,M}\sqrt{\frac{2\ell+1}{2L+1}}\,c_{1,0,\ell,0}^{L,0}c_{1,0,\ell,m}^{L,M}\, Y_L^M(\theta,\varphi)\ , \tag{101c}$$

where $c_{\ell',m',\ell,m}^{L,M}$ are the Clebsch–Gordan coefficients, further detailed [42] in appendix B.

The coupling matrix $W_{\ell',\ell}^{m',m}(\mathbf{k})$ can therefore be written as

$$W_{\ell',\ell}^{m',m}(\mathbf{k}) = W_{\ell',\ell}^{m',m}(k_x\mathbf{e}_x) + W_{\ell',\ell}^{m',m}\left(k_y\mathbf{e}_y\right) + W_{\ell',\ell}^{m',m}(k_z\mathbf{e}_z)\,. \tag{102}$$

the simplest among the three terms is

$$W_{\ell',\ell}^{m',m}(k_z\mathbf{e}_z) = -\mathring{\imath}w_0 k_z\sum_{L,M}\sqrt{\frac{2\ell+1}{2L+1}}\,c_{1,0,\ell,0}^{L,0}c_{1,0,\ell,m}^{L,M}\delta_{m',M}\delta_{\ell',L} \tag{103a}$$

$$= -\mathring{\imath}w_0 k_z\delta_{m,m'}\left\{\sqrt{\frac{(\ell+1+m)(\ell+1-m)}{(2\ell+1)(2\ell+3)}}\delta_{\ell',\ell+1} + \sqrt{\frac{(\ell+m)(\ell-m)}{(2\ell+1)(2\ell-1)}}\delta_{\ell',\ell-1}\right\}\ , \tag{103b}$$

with the other two stated in appendix B. With this framework in place, we proceed to calculate the MSD and the density at stationarity.

3.2.1. MSD

We follow section 2.2.1 to calculate the MSD of ABPs in three dimensions, which is

$$\overline{\mathbf{r}^2}(t-t_0) = 3\overline{z^2}(t-t_0)$$
$$= -3\,\partial_{k_z}^2\big|_{\mathbf{k}=0}\int_0^{\pi}\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\varphi\,\sin\theta\,\frac{1}{4\pi}\int_0^{\pi}\mathrm{d}\theta_0\int_0^{2\pi}\mathrm{d}\varphi_0\,\sin\theta_0\int\mathrm{đ}^3k_0\,\left\langle\chi(\mathbf{k},\theta,\varphi,t)\,\tilde{\chi}(\mathbf{k}_0,\theta_0,\varphi_0,t_0)\right\rangle \tag{104}$$

corresponding to equation (57). With the help of the diagrammatics equation (56) and the reasoning before equation (58), this can essentially be done by inspection. The derivative of the bare propagator will contribute $-3(-2\mathsf{D}_t t)$ to the MSD. The only non-trivial contribution is due to , which has a very simple structure because the integration over θ and φ, forces $\ell=0$ and $m=0$, given that Y_ℓ^m are orthogonal and $Y_0^0 = 1/\sqrt{4\pi}$ and so integrals over Y_ℓ^m vanish unless $\ell = m = 0$. The same reasoning applies to $\ell_0 = m_0 = 0$. The summation that appears in the last term of equation (56) therefore becomes

$$\sum_{\ell_1=0}^{\infty}\sum_{m_1=-\ell_1}^{\ell_1} W_{0,\ell_1}^{0,m_1}(k_z\mathbf{e}_z)H_{\ell_1}^{m_1}(k_z\mathbf{e}_z,\omega)\,W_{\ell_1,0}^{m_1,0}(k_z\mathbf{e}_z) = -w_0^2k_z^2\frac{1}{3}\frac{1}{-\imath\omega+\mathsf{D}_tk_z^2+2\mathsf{D}_r} \tag{105}$$

because only $\ell_1 = 1$ contributes, resulting in a factor $\ell_1(\ell_1+1) = 2$ in front of D_r in the propagator. Differentiating twice with respect to k_z and taking the inverse Fourier transform of the expression with the bare propagators attached,

$$-\frac{2}{3}w_0^2\lim_{m\downarrow 0}\int\mathrm{đ}\,\omega\,\mathrm{e}^{-\imath\omega t}\frac{1}{(-\imath\omega+\mu)^2}\frac{1}{-\imath\omega+2\mathsf{D}_r+\mu} = \frac{2}{3}w_0^2\left\{\frac{-t}{2\mathsf{D}_r}+\frac{1}{4\mathsf{D}_r^2}-\frac{1}{4\mathsf{D}_r^2}\mathrm{e}^{-2\mathsf{D}_r t}\right\} \tag{106}$$

finally reproduces equation (81) exactly.

3.2.2. External potential

Calculating the stationary density $\rho_0(\mathbf{r})$ in the presence of an external potential perturbatively in the self-propulsion and the potential follows the pattern outlined in section 2.2.2. Because the volume is finite, the representation we choose for the fields is

$$\chi(\mathbf{r},\varphi,t) = \int\mathrm{đ}\,\omega\,\frac{1}{L^3}\sum_{\mathbf{n}\in\mathbb{Z}^3}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\mathrm{e}^{-\imath\omega t}\mathrm{e}^{\imath\mathbf{k_n}\cdot\mathbf{r}}(4\pi)^{1/2}\,Y_\ell^m(\theta,\varphi)\,\chi_\ell^m(\mathbf{k_n},\omega) \tag{107a}$$

$$\tilde{\chi}(\mathbf{r},\varphi,t) = \int\mathrm{đ}\,\omega\,\frac{1}{L^3}\sum_{\mathbf{n}\in\mathbb{Z}^3}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\mathrm{e}^{-\imath\omega t}\mathrm{e}^{\imath\mathbf{k_n}\cdot\mathbf{r}}(4\pi)^{-1/2}\,(Y_\ell^m(\theta,\varphi))^*\,\tilde{\chi}_\ell^m(\mathbf{k_n},\omega)\ . \tag{107b}$$

rather than equation (93), with the sums over $\mathbf{n}\in\mathbb{Z}^3$ replacing the integrals over $\mathbf{k}$.

Given the orthogonality of the spherical harmonics, the perturbative part of the action now reads

$$\mathcal{A}_{P2} = \int\mathrm{đ}\,\omega\,\frac{1}{L^6}\sum_{\mathbf{n}_1,\mathbf{n}_2}\sum_{\ell,\ell'=0}^{\infty}\sum_{m=-\ell}^{\ell}\sum_{m'=-\ell'}^{\ell'}\chi_\ell^m(\mathbf{k}_{\mathbf{n}_1},\omega)\,\tilde{\chi}_{\ell'}^{m'}(\mathbf{k}_{\mathbf{n}_2},-\omega)\,\delta_{\mathbf{n}_1+\mathbf{n}_2,\mathbf{0}}W_{\ell',\ell}^{m',m}(\mathbf{k}_{\mathbf{n}_1})$$
$$+\frac{1}{L^9}\sum_{\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3}L^3\delta_{\mathbf{n}_1+\mathbf{n}_2+\mathbf{n}_3,\mathbf{0}}\sum_{\ell_1,\ell_3}\sum_{m=-\ell_3}^{\ell_3}\sum_{m'=-\ell_1}^{\ell_1}(\mathbf{k}_{\mathbf{n}_1}\cdot\mathbf{k}_{\mathbf{n}_2})\,\tilde{\chi}_{\ell_1}^{m'}(\mathbf{k}_{\mathbf{n}_1},-\omega)\,\Upsilon_{\mathbf{n}_2}\chi_{\ell_3}^m(\mathbf{k}_{\mathbf{n}_3},\omega) \tag{108}$$

corresponding to equation (60) in two dimensions, but with the coupling vertex $W_{\ell',\ell}^{m',m}(\mathbf{k})$ given by equation (100).

In principle, $\Upsilon_\mathbf{n}$ is arbitrary, but in order to stay with the simple form of $W_{\ell',\ell}^{m',m}(k_z\mathbf{e}_z)$, equation (103b), we restrict $\Upsilon(\mathbf{r})$ to vary only with z, making again use of the notation equation (87). The sole contribution that needs our attention is due to the single term equation (65), which draws on equation (105): If the modes of the external potential $\Upsilon_\mathbf{n}$ vanish for $\mathbf{k_n}\not\parallel\mathbf{e}_z$ in the diagram equation (65), the x and the y components of $\mathbf{k_n}$ and $\mathbf{k_p}$ have to cancel. As $t_0\to-\infty$ effectively enforces $\mathbf{k_p}=\mathbf{0}$, this means that equation (65) vanishes in this limit for any $\mathbf{k_n}\not\parallel\mathbf{e}_z$, so that $W_{\ell',\ell}^{m',m}(\mathbf{k_n})$ is only ever evaluated in the simplest case $W_{\ell',\ell}^{m',m}(k_z\mathbf{e}_z)$, equation (103b).

Using $W^{0,0}_{0,1}(k_z\mathbf{e}_z)W^{0,0}_{1,0}(k_z\mathbf{e}_z) = -w_0^2k_z^2/3$, the density can be read off equation (68*b*)

$$\rho_0(\mathbf{r}) = L^{-3} - \frac{1}{L^4}\sum_{n_z\neq 0} \mathrm{e}^{\mathring{\imath}k_{n_z}z}\frac{\Upsilon_{n_z}}{\mathsf{D}_t}\left\{1 - \frac{w_0^2}{3\mathsf{D}_t}\left(\mathsf{D}_t k_{n_z}^2 + 2\mathsf{D}_r\right)^{-1}\right\} + \mathcal{O}\left(w_0^4\right) + \ldots \tag{109}$$

with the denominator of the fraction $w_0^2/(3\mathsf{D}_t)$ changed from $w_0^2/(2\mathsf{D}_t)$ in equation (68*b*), and the internal propagator changed to $(\mathsf{D}_tk_{n_z}^2 + 2\mathsf{D}_r)^{-1}$ from $(\mathsf{D}_tk_{\mathbf{n}}^2 + \mathsf{D}_r)^{-1}$. Comparing to equations (C20) and (109) reveals corrections to order w_0^2 in the form $w_0^2/(3\mathsf{D}_t(\mathsf{D}_tk_{n_z}^2 + 2\mathsf{D}_r))$ and higher beyond replacing D_t at $\mathbf{w}_0 = \mathbf{0}$ in equation (C20) by $\mathsf{D}^{3\mathrm{D}}_{\mathrm{eff}}$ equation (82).

Equation (109) correctly reproduces the result based on the expansion in 'three-dimensional Mathieu functions', equation (91), as

$$1 - \frac{w_0^2}{3\mathsf{D}_t}\left(\mathsf{D}_tk_{n_z}^2 + 2\mathsf{D}_r\right)^{-1} + \mathcal{O}\left(w_0^4\right) = \mathsf{D}_t\left\{\left(\mathsf{D}_t + w_0^2/(6\mathsf{D}_r) + \mathcal{O}\left(q^4\right)/k_{n_z}^2\right)^{-1} + \frac{k_{n_z}^4 w_0^2}{12\mathsf{D}_r^2}\left[\left(\mathsf{D}_tk_{n_z}^2 + w_0^2k_{n_z}^2/(6\mathsf{D}_r) + \mathcal{O}\left(q^4\right)\right)^{-1} - \left(\mathsf{D}_tk_{n_z}^2 + 2\mathsf{D}_r + \mathsf{D}_r\mathcal{O}\left(q^2\right)\right)^{-1}\right]\right\}. \tag{110}$$

4. Discussion and conclusion

There are two main perspectives on the present results, first about the concrete observables calculated and second about the formalism.

4.1. Observables

In this work we calculated the MSD and the stationary density of ABPs in two and three dimensions using two distinct methods. The MSD calculations were performed primarily for methodological purposes, and the field-theoretic derivation of the full time-dependence of the MSD of a free ABP in three dimensions, but not in two [11], is a new result, whereas the MSD itself is well-known [2, 3, 9, 11].

In two dimensions, we determined the exact MSD of ABPs using Mathieu functions with full time dependence in equation (28) as well as using the perturbative approach leading to equation (59). In three dimensions, similarly to the two-dimensional case, we used 'three-dimensional Mathieu functions' for computation of the exact full time-dependent MSD in equation (81) and spherical harmonics in equation (106). The effective diffusion constants for both, the two and three-dimensional case in equations (29) and (82) respectively, are identical to the RnT motion case using appropriate conversion [3, 11].

The MSD was calculated irrespective of the final orientation of the ABP and integrated about the initial angle without loss of generality. This leads to a significant reduction in the number of terms in the final MSD expression as discussed after equation (23) in two dimensions. The same method was used in the three-dimensional case with 'three-dimensional Mathieu functions' in section 3.1.1. For the self-propulsion perturbative case, it is a matter of convenience to determine the MSD in only one spatial direction, which however requires uniform initialisation in order to avoid bias, as discussed in two dimensions after equation (61). The same approach was taken in three dimensions in section 3.2.1. Generalising to $d > 3$ dimensions using the perturbative approach and so-called hyperspherical harmonics [43, 44], the expression for the MSD of ABPs is [44]

$$\overline{\mathbf{r}^2}(t) = 2dDt + \frac{2w_0^2}{(d-1)^2D_r^2}\left(\mathrm{e}^{-(d-1)D_rt} - 1 + (d-1)D_rt\right). \tag{111}$$

with the details to be found in [45]. The effective diffusion constant

$$\mathsf{D}^{d\mathrm{D}}_{\mathrm{eff}} = D + \frac{w_0^2}{d(d-1)D_r} \quad \text{for} \quad d \geqslant 2 \tag{112}$$

is consistent with [3].

The calculation of the stationary density in the presence of the external potential is, to our knowledge, a new result with the present generality. The stationary density in two dimensions was computed perturbatively in presence of small potentials in equations (46), (48) and (68) to first order in the potential. These expressions differ only in that they are expanded in different parameters, i.e. the parameter q of the Mathieu function in (46), the spatial momentum $\mathbf{k}_n$ in (48) and $\mathbf{k}, w_0$ in (68). We further assumed a finite volume L^d, to guarantee a stationary state in the absence of a potential, similar to drift-diffusive case discussed in appendix C. As a result of using Fourier sums, the potentials and the resulting observables are periodic. The two-dimensional MSD is in agreement with experimental results [1, 46].

In three dimensions, the stationary density calculation with the 'three-dimensional Mathieu-functions' in the external potential was simplified by allowing the potential to vary in only one direction, equation (87), appendix A. Although the calculations without this assumption are much richer and much messier, we do not believe that they produce results that are qualitatively much different from those presented here. In two dimensions, this assumption was avoided by the re-orientation of the coordinate system in section 2.1. In the perturbative approach, section 3.2, the above-mentioned assumption helped avoid having to compute general Clebsch–Gordan coefficients in equation (100), but determined nevertheless in appendix B.

The stationary density in three dimensions in equation (91) is calculated to first order in the potential and expanded to second order in $\mathbf{q}$. The perturbative calculation in the self-propulsion results in equation (109). The restriction on the potential in three dimensions is more easily lifted in the perturbation theory using spherical harmonics, since the Clebsch–Gordan coefficients can be derived without much ado. On the other hand, characterising the 'three-dimensional Mathieu functions' requires at the very least a careful analysis of the completeness of the eigensystem, more easily done for $\mathbf{q} \parallel \mathbf{e}_z$.

Despite the restrictions on the potential, the perturbation theory covers a wide class of potentials. As is analysed in detail for drift-diffusive systems in appendix C, the resummed pertubation theory recovers known closed form expressions, including a confining potential. The most interesting case of 'active sedimentation' in a gravitational potential in a finite vessel can be realised within the restrictions mentioned above by long-stretched, periodic ratchet in the z-direction with period L,

$$\Upsilon(\mathbf{r}) = \mu_p m g \mathbf{r} \cdot \mathbf{e}_z \tag{113}$$

with particle mass m, gravitational acceleration g and mobility μ_p. With $\mathbf{r}$ confined to $[0, L)^d$ by periodicity, $\mathbf{r} \cdot \mathbf{e}_z = -\epsilon L$ with $\epsilon \in [0, 1)$ is mapped to $\Upsilon((1-\epsilon)L\mathbf{e}_z)$ by periodicity in equation (32), so that the potential 'energy' equation (113) jumps to the maximum right after reaching the minimum for decreasing z, implementing a sharp potential wall at $z = 0$, the bottom of the vessel. The corresponding modes of the potential are $\Upsilon_{n_z} = \mathring{\imath} L/k_{n_z}$ for $n_z \neq 0$, and $L/2$ for $n_z = 0$, to be used in equation (91) or (109), but not in the expansion in small $\mathbf{k_n}$, equation (92), as discussed after equation (48).

The 'barometric formulas' in equations (48) and (92) show the corrections to the density that are generically due to the activity. Those cannot possibly affect the 0-mode, which is explicitly excluded from the summation. To leading order the density of ABPs behaves like that of an equilibrium system with no self-propulsion, $\mathbf{w}_0 = \mathbf{0}$ and the translational diffusion constant D_t, equation (C20), replaced by the effective diffusion constant D_{eff}, equations (29) and (82). Terms beyond that are generically due to the non-equilibrium nature of active matter. The lowest order correction is quadratic in $k_{\mathbf{n}}$, namely $w_0^2 k_{\mathbf{n}}^2/(2\mathsf{D}_r^2)$ in two dimensions and $w_0^2 k_{\mathbf{n}}^2/(12\mathsf{D}_r^2)$ in three dimensions. It might be interesting to investigate how this can be measured in slowly varying potentials where contributions in large $\mathbf{n}$ are suppressed because $\Upsilon_{\mathbf{n}}$ vanishes there. The experimental studies and data known to us [1, 39, 46–51] confirm the presence of the effective diffusion constant, but are not detailed enough to reveal the $k_{\mathbf{n}}$-dependent corrections that we have determined here.

4.2. Methodology

We have introduced all ingredients to set up a field theory of ABPs, in particular: the action, the propagators, the projections of the special functions such as $\Delta_{\ell_1,\ell_3}(-\mathbf{k}_{\mathbf{n}_1}, -\mathbf{k}_{\mathbf{n}_3})$, equations (33) and (85)), and the coupling vertices (such as $W_{\ell',\ell}(\mathbf{k})$, equations (54*a*) and (100). As well as providing the concrete mathematical framework, our derivations above highlight the advantages and disadvantages of using special functions rather than a perturbation theory. We will briefly summarise these here.

Using *special functions*, i.e. the Mathieu functions, sections 2.1 and 3.1, has the benefit that the bare propagator already contains the self-propulsion. As long as space $\mathbf{r}$ and its boundary conditions can be implemented through a Fourier-transform, this is the most efficient way to deal with *free* problems, wrapping the self-propulsion in the properties of certain special functions. The resulting bare propagator is the exact and complete characterisation of the free stochastic particle movement. When the special functions are well-known, literature provides the relevant properties of functions and eigenvalues. When they are not well-known, they can be determined *perturbatively* in (hyper-)spherical harmonics, effectively performing the perturbation theory that would otherwise be done explicitly at the level of diagrams. In return, the wealth of literature on Sturm–Liouville problems is readily applicable, as touched on in equation (A8).

We were able to avoid having to determine the 'three-dimensional Mathieu functions' in greater detail by using a preferred direction, which generally requires integration of final and/or initial orientation. Thanks to the arbitrary function $\sigma(\mathbf{k})$ in equation (13), this was avoided two dimensions, where we could use the well-known Mathieu functions. This may be related to the metric of a d-dimensional sphere to be curved only in $d > 2$. In three dimensions, despite having *two* arbitrary functions $\sigma(\mathbf{k})$ and $\tau(\mathbf{k})$ in equation (72), an elegant simplification of the eigenproblem does not seem to be available.

Using a *perturbation theory*, i.e. expanding diagrams in w_0, sections 2.2 and 3.2, means that even the free particle has to be treated explicitly perturbatively. Although the full propagator now contains infinitely many terms, this does necessarily translate to infinitely many terms for every observable, as seen, for example, in the fully time-dependent MSD calculated exactly using perturbation theory in two and three dimensions, sections 2.2.1 and 3.2.1 respectively. The big advantage of using a perturbation theory is that orthogonality is not spoiled by a lack of momentum conservation, as is caused by an external potential or interaction. Such a lack of momentum conservation is what necessitates the introduction of the projection $\Delta_{\ell_1,\ell_3}(-\mathbf{k}_{\mathbf{n}_1},-\mathbf{k}_{\mathbf{n}_3})$ in the case of special functions, equation (34) and similarly (84), but this does not happen when using a perturbation theory, equations (60) and (108).

It is striking that the perturbation theory in weak potentials recovers the barometric formula for a binding potential (appendix C). The calculation of such stationary features is facilitated by the amputation mechanism as discussed in section 2.1.2 and similarly used in [11].

4.3. Outlook

We are currently working on a field theory of *interacting* ABPs displaying features of the Vicsek Model [12, 13, 19–21]. As the upper critical dimension there is $d_c = 4$, we aim to generalise the spherical harmonics to higher dimensions. This would also allow the use of dimensional regularisation in a renormalised field theory. While some characteristics of such hyperspherical functions follow a systematic pattern, allowing the spatial dimension to vary continuously like $d = 4 - \epsilon$ represents a significant challenge.

Data availability statement

No new data were created or analysed in this study.

Acknowledgments

The authors would like to thank Wilson Poon for providing relevant material. We also thank Rosalba Garcia-Millan for her hint on Mathieu functions.

Appendix A. Three-dimensional Mathieu functions

In the following, we want to characterise the 'three-dimensional Mathieu functions', which we call that only because the eigenfunctions of the equations below in two dimensions are the well-known Mathieu-functions [32, 33].

We will first state the defining equations and then set out to calculate the eigenfunctions. Firstly, we demand that $u_\ell^m(\theta,\varphi,\mathbf{q})$ are eigenfunctions, equation (76)

$$\left(-\mathbf{q}\cdot\begin{pmatrix}\sin\theta\cos\varphi\\ \sin\theta\sin\varphi\\ \cos\theta\end{pmatrix}+\frac{1}{\sin\theta}\partial_\theta\sin\theta\,\partial_\theta+\frac{1}{\sin^2\theta}\partial_\varphi^2\right)u_\ell^m(\theta,\varphi,\mathbf{q})=-\lambda_\ell^m(\mathbf{q})\,u_\ell^m(\theta,\varphi,\mathbf{q})\ . \tag{A1}$$

Further, we demand normalisation,

$$\int_0^\pi \mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\varphi\,\sin\theta\,u_\ell^m(\theta,\varphi,\mathbf{q})\,u_{\ell'}^{m'}(\theta,\varphi,\mathbf{q})=\delta_{\ell,\ell'}\delta_{m,m'} \tag{A2}$$

with equation (73) to maintain close correspondence to the two-dimensional case equation (26),

$$\widetilde{u}_\ell^m(\theta,\varphi,\mathbf{q}(\mathbf{k}))=\frac{1}{4\pi}u_\ell^m(\theta,\varphi,\mathbf{q}(\mathbf{k})) \tag{A3}$$

and orthogonality following from the self-adjointness of the differential operator equation (A1) under the scalar product equation (A2). With that, all of Sturm–Liouville theory [52] is at our disposal. We will index these eigenfunctions with $\ell = 0, 1, \ldots$ and $m \in \mathbb{Z}$.

For $\mathbf{q}=\mathbf{0}$ vanishing, equation (A1) is the eigen-equation of the spherical harmonics [32]. We therefore choose to express the three-dimensional Mathieu functions in spherical harmonics $Y_j^k(\theta,\varphi)$,

$$u_\ell^m(\theta,\varphi,\mathbf{q}) = \sqrt{4\pi}\sum_{j=0}^{\infty}\sum_{k=-j}^{j} A_{\ell,j}^{m,k}(\mathbf{q})\,Y_j^k(\theta,\varphi) = \sum_{j=0}^{\infty}\sum_{k=-j}^{j} A_{\ell,j}^{m,k}(\mathbf{q})\sqrt{\frac{(2j+1)(j-k)!}{(j+k)!}}P_j^k(\cos\theta)\,\mathrm{e}^{\mathring{\imath}k\varphi} \tag{A4}$$

with the factor of $\sqrt{4\pi}$ solely to ease notation and $P_\ell^m(z)$ denoting the associated Legendre polynomials. For $\mathbf{q}=\mathbf{0}$, $A_{\ell,j}^{m,k}(\mathbf{q})$ is diagonal, so that

$$A_{\ell,j}^{m,k}(\mathbf{q}) = \left(\delta_{\ell,j}\delta_{m,k}+\mathcal{O}(\mathbf{q})\right) \tag{A5a}$$

$$\lambda_\ell^m(\mathbf{q}) = \ell(\ell+1)+\mathcal{O}(\mathbf{q})\ , \tag{A5b}$$

where we assume that the coefficients $A_{\ell,j}^{m,k}(\mathbf{q})$ and eigenvalues $\lambda_\ell^m(\mathbf{q})$ can be expanded in small $\mathbf{q}$. Explicitly, for $\mathbf{q}=\mathbf{0}$,

$$u_\ell^m(\theta,\varphi,\mathbf{0}) = \sqrt{4\pi}Y_\ell^m(\theta,\varphi) \tag{A6a}$$

$$u_\ell^m(\theta,\varphi,\mathbf{0}) = \frac{1}{\sqrt{4\pi}}\left(Y_\ell^m(\theta,\varphi)\right)^*\ , \tag{A6b}$$

with the asterisk denoting the complex conjugate and indeed

$$\int_0^\pi \mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\varphi\,\sin\theta u_\ell^m(\theta,\varphi,\mathbf{0})\,\tilde{u}_{\ell'}^{m'}(\theta,\varphi,\mathbf{0}) = \delta_{\ell,\ell'}\delta_{m,m'}\ . \tag{A7}$$

We focus henceforth on those $\mathbf{q}$ that have no projection in the x and y directions, $\mathbf{q}=(0,0,q)^\mathsf{T}=q\mathbf{e}_z$, which simplifies equation (A1) dramatically, rendering it similar to the expression in two dimensions, equation (19). Only the θ-dependence is affected by the presence of $\mathbf{q}\parallel\mathbf{e}_z$, so that $A_{\ell,j}^{m,k}(\mathbf{q})\propto\delta_{m,k}$ is diagonal in m,k for such $\mathbf{q}$, resulting in a simple structure and indexing of the azimuthal dependence, i.e. on φ,

$$u_\ell^m(\theta,\varphi,\mathbf{q}(k_z\mathbf{e}_z)) = \mathrm{e}^{\mathring{\imath}m\varphi}\sum_{j=0}^{\infty}A_{\ell,j}^{m,m}(q\mathbf{e}_z)\sqrt{\frac{(2j+1)(j-m)!}{(j+m)!}}P_j^m(\cos\theta)\ . \tag{A8}$$

Because we will integrate $u_\ell^m(\theta,\varphi,\mathbf{q}(k_z\mathbf{e}_z))$ over φ, we can further narrow down the scope of this section to $m=0$, which simplifies the square root in equation (A8) to $\sqrt{2j+1}$.

Because the Legendre polynomials obey

$$cos\theta P_\ell^m = \frac{\ell-m+1}{2\ell+1}P_{\ell+1}^m+\frac{\ell+m}{2\ell+1}P_{\ell-1}^m\ , \tag{A9}$$

the eigen-equation equation (A1) for $m=0$ and $\mathbf{q}=q\mathbf{e}_z$ with equation (A4) is simply

$$0=\sum_{j=0}^{\infty}A_{\ell,j}^{0,0}(q\mathbf{e}_z)\sqrt{2j+1}\left(q\frac{j+1}{2j+1}P_{j+1}^0(\cos\theta)+q\frac{j}{2j+1}P_{j-1}^0(\cos\theta)+\left(j(j+1)-\lambda_\ell^0(q\mathbf{e}_z)\right)P_j^0(\cos\theta)\right)\ . \tag{A10}$$

Projecting out the Legendre polynomials one by one, the coefficients $A_{\ell,j}^{0,0}(q\mathbf{e}_z)$ obey

$$0=\alpha_{\ell,j-1}q\frac{j}{\sqrt{2j-1}}+\alpha_{\ell,j+1}q\frac{j+1}{\sqrt{2j+3}}+\alpha_{\ell,j}\sqrt{2j+1}\left(j(j+1)-\lambda_\ell^0\right) \tag{A11}$$

where we have used

$$\alpha_{\ell,j}=\mathcal{N}_\ell^0A_{\ell,j}^{0,0}(q\mathbf{e}_z)\ , \tag{A12}$$

with some normalisation $\mathcal{N}_\ell^0$ to be used below, and $\lambda_\ell=\lambda_\ell^0(q\mathbf{e}_z)$ to ease notation.

Equation (A11) can of course be written in matrix form

$$\begin{pmatrix} 0 & \frac{q}{\sqrt{3}} & 0 & \\ \frac{q}{\sqrt{3}} & 2 & \frac{2q}{\sqrt{15}} & \cdots \\ 0 & \frac{2q}{\sqrt{15}} & 6 & \\ & \vdots & & \ddots \end{pmatrix}\begin{pmatrix}\alpha_{\ell,0}\\ \alpha_{\ell,1}\\ \alpha_{\ell,2}\\ \vdots\end{pmatrix} = \lambda_\ell^0(q\mathbf{e}_z)\begin{pmatrix}\alpha_{\ell,0}\\ \alpha_{\ell,1}\\ \alpha_{\ell,2}\\ \vdots\end{pmatrix}. \tag{A13}$$

By demanding that this equation is to be solved to a certain order in q and by *assuming* $\alpha_{\ell,j}\in\mathcal{O}\left(q^{|\ell-j|}\right)$, only a finite number of matrix elements and vector elements need to be considered at a time, while also constraining the order of the eigenvalue. Using equation (A5) as the starting point, the first order equation for $\ell=0$ is

$$\begin{pmatrix} 0 & \frac{q}{\sqrt{3}} \\ \frac{q}{\sqrt{3}} & 2 \end{pmatrix}\begin{pmatrix} 1 \\ u_1 q \end{pmatrix} = (0+vq)\begin{pmatrix} 1 \\ u_1 q \end{pmatrix} + \mathcal{O}\left(q^2\right) , \tag{A14}$$

where we have labelled the unknown term of $\alpha_{0,1}$ by $u_1 q$ and the unknown term of $\lambda_0^0(q\mathbf{e}_z)$ by vq. The 0 in the eigenvalue on the right hand side of equation (A14) is that of λ_ℓ^0 at $\ell=0$, equation (A5*b*). Focussing solely on terms of order q produces two equations, $0=vq$ and $q/\sqrt{3}+2u_1q=0$, determining both $v=0$ and $u_1=-1/(2\sqrt{3})$. With those in place, the next order equation is

$$\begin{pmatrix} 0 & \frac{q}{\sqrt{3}} & 0 \\ \frac{q}{\sqrt{3}} & 2 & \frac{2q}{\sqrt{15}} \\ 0 & \frac{2q}{\sqrt{15}} & 6 \end{pmatrix}\begin{pmatrix} 1 \\ -\frac{q}{2\sqrt{3}}+u_1q^2 \\ u_2q^2 \end{pmatrix} = \left(0+vq^2\right)\begin{pmatrix} 1 \\ -\frac{q}{2\sqrt{3}}+u_1q^2 \\ u_2q^2 \end{pmatrix} + \mathcal{O}\left(q^3\right) , \tag{A15}$$

determining u_1, u_2 and v, now labelling terms of order q^2.

The only additional difficulty for $\ell>0$ is that the number of rows and columns of the matrix to be considered going from one order to the next may increase by 2 for the first ℓ orders. For example the first non-trivial order for $\ell=1$ is

$$\begin{pmatrix} 0 & \frac{q}{\sqrt{3}} & 0 \\ \frac{q}{\sqrt{3}} & 2 & \frac{2q}{\sqrt{15}} \\ 0 & \frac{2q}{\sqrt{15}} & 6 \end{pmatrix}\begin{pmatrix} u_0q \\ 1 \\ u_2q \end{pmatrix} = (2+vq)\begin{pmatrix} u_0q \\ 1 \\ u_2q \end{pmatrix} + \mathcal{O}\left(q^2\right) . \tag{A16}$$

With this process, we have determined

$$\left[\begin{pmatrix} 0 & \frac{q}{\sqrt{3}} & 0 & 0 & 0 \\ \frac{q}{\sqrt{3}} & 2 & \frac{2q}{\sqrt{15}} & 0 & 0 \\ 0 & \frac{2q}{\sqrt{15}} & 6 & \frac{3q}{\sqrt{35}} & 0 \\ 0 & 0 & \frac{3q}{\sqrt{35}} & 12 & \frac{4q}{\sqrt{63}} \\ 0 & 0 & 0 & \frac{4q}{\sqrt{63}} & 20 \end{pmatrix} - \left(-\frac{q^2}{6}+\frac{11q^4}{1080}\right)\mathbb{1}\right]\begin{pmatrix} 1 \\ -\frac{q}{2\sqrt{3}}+\frac{11q^3}{360\sqrt{3}} \\ \frac{q^2}{18\sqrt{5}}-\frac{43q^4}{9072\sqrt{5}} \\ -\frac{q^3}{360\sqrt{7}} \\ \frac{q^4}{37800} \end{pmatrix} \in \mathcal{O}\left(q^5\right) \qquad \text{for } \ell=0 , \tag{A17}$$

which can be improved further by demanding that the term of order q^6 in λ_0^0 is consistent with $\alpha_{0,2}=q^2/(18\sqrt{5})-43q^4/(9072\sqrt{5})$ in equation (A17), producing

$$\lambda_0^0(q\mathbf{e}_z) = -\frac{q^2}{6}+\frac{11q^4}{1080}-\frac{47q^6}{34020}+\mathcal{O}\left(q^7\right) \qquad \text{for } \ell=0 . \tag{A18}$$

For $\ell=1$, we found

$$\left[\begin{pmatrix} 0 & \frac{q}{\sqrt{3}} & 0 & 0 & 0 \\ \frac{q}{\sqrt{3}} & 2 & \frac{2q}{\sqrt{15}} & 0 & 0 \\ 0 & \frac{2q}{\sqrt{15}} & 6 & \frac{3q}{\sqrt{35}} & 0 \\ 0 & 0 & \frac{3q}{\sqrt{35}} & 12 & \frac{4q}{\sqrt{63}} \\ 0 & 0 & 0 & \frac{4q}{\sqrt{63}} & 20 \end{pmatrix} - \left(2+\frac{q^2}{10}\right)\mathbb{1}\right]\begin{pmatrix} \frac{q}{2\sqrt{3}}-\frac{q^3}{40\sqrt{3}} \\ 1 \\ -\frac{q}{2\sqrt{15}}-\frac{11q^3}{700\sqrt{15}} \\ \frac{3q^2}{100\sqrt{21}} \\ -\frac{q^3}{3150\sqrt{3}} \end{pmatrix} \in \mathcal{O}\left(q^4\right) \qquad \text{for } \ell=1 , \tag{A19}$$

i.e.

$$\lambda_1^0(q\mathbf{e}_z) = 2+\frac{q^2}{10}+\mathcal{O}\left(q^4\right) \qquad \text{for } \ell=1 . \tag{A20}$$

Matrix expressions such as equations (A17) and (A19) are easily verified with a computer algebra system, simply by determining whether the remainder has the expected order.

Equations (A2) and (A4) imply

$$\sum_{j=0}^{\infty}\sum_{k=-j}^{j}\left(A_{\ell,j}^{m,k}\left(q\mathbf{e}_z\right)\right)^2=1 \tag{A21}$$

which determines the normalization $\mathcal{N}_\ell^0$ in equation (A12) and with equation (A17) this produces the desired coefficients for $\ell=0$,

$$A_{0,0}^{0,0}\left(q\mathbf{e}_z\right)=1-\frac{q^2}{24}+\frac{383q^4}{51840}+\mathcal{O}\left(q^5\right) \tag{A22a}$$

$$A_{0,1}^{0,0}\left(q\mathbf{e}_z\right)=-\frac{q}{2\sqrt{3}}+\frac{37q^3}{720\sqrt{3}}+\mathcal{O}\left(q^5\right) \tag{A22b}$$

$$A_{0,2}^{0,0}\left(q\mathbf{e}_z\right)=\frac{q^2}{18\sqrt{5}}-\frac{4q^4}{567\sqrt{5}}+\mathcal{O}\left(q^5\right) \tag{A22c}$$

$$A_{0,3}^{0,0}\left(q\mathbf{e}_z\right)=-\frac{q^3}{360\sqrt{7}}+\mathcal{O}\left(q^5\right) \tag{A22d}$$

$$A_{0,4}^{0,0}\left(q\mathbf{e}_z\right)=\frac{q^4}{37800}+\mathcal{O}\left(q^5\right)\ . \tag{A22e}$$

Similarly, we found for $\ell=1$ from equation (A19),

$$A_{1,0}^{0,0}\left(q\mathbf{e}_z\right)=\frac{q}{2\sqrt{3}}-\frac{q^3}{20\sqrt{3}}+\mathcal{O}\left(q^4\right) \tag{A23a}$$

$$A_{1,1}^{0,0}\left(q\mathbf{e}_z\right)=1-\frac{q^2}{20}+\mathcal{O}\left(q^4\right) \tag{A23b}$$

$$A_{1,2}^{0,0}\left(q\mathbf{e}_z\right)=-\frac{q}{2\sqrt{15}}+\frac{13q^3}{1400\sqrt{15}}+\mathcal{O}\left(q^4\right) \tag{A23c}$$

$$A_{1,3}^{0,0}\left(q\mathbf{e}_z\right)=\frac{1}{100}\sqrt{\frac{3}{7}}q^2+\mathcal{O}\left(q^4\right)\ . \tag{A23d}$$

For general ℓ we observe that in deed

$$A_{\ell,0}^{0,0}\left(q\mathbf{e}_z\right)\in\mathcal{O}\left(q^\ell\right) \tag{A24}$$

by construction.

Finally, we calculate the integral of $u_\ell^m(\theta,\varphi,\mathbf{q}(q\mathbf{e}_z))$ over φ and θ, equation (79). Firstly, taking the integral over φ of the definition equation (A8) enforces $m=0$,

$$\int_0^\pi \mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\varphi\ \sin\theta u_\ell^m\left(\theta,\varphi,\mathbf{q}\left(\mathbf{k}\right)\right)=2\pi\,\delta_{m,0}\sum_{j=0}^{\infty}A_{\ell,j}^{0,0}\left(\mathbf{q}\left(\mathbf{k}\right)\right)\sqrt{2j+1}\int_0^\pi\mathrm{d}\theta\ \sin\theta\, P_j^0\left(\cos\theta\right)\ . \tag{A25}$$

Using the orthogonality of the Legendre polynomials,

$$\int_0^\pi\mathrm{d}\theta\ \sin\theta\, P_j^m\left(\cos\theta\right)P_k^m\left(\cos\theta\right)=\frac{2\left(j+m\right)!}{\left(2j+1\right)\left(j-m\right)!}\delta_{j,k} \tag{A26}$$

and $P_0^0=1$, which means that the integral of P_j^0 is its projection against $P_0^0=1$, then gives the desired

$$\int_0^\pi\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\varphi\ \sin\theta u_\ell^m\left(\theta,\varphi,\mathbf{q}\left(\mathbf{k}\right)\right)=4\pi\,\delta_{m,0}A_{\ell,0}^{0,0}\left(\mathbf{q}\left(\mathbf{k}\right)\right)\ . \tag{A27}$$

Appendix B. Clebsch–Gordan coefficients

A product of two spherical harmonics can be expanded as

$$Y_\ell^m\left(\theta,\varphi\right)Y_{\ell'}^{m'}\left(\theta,\varphi\right)=\sum_{L,M}\sqrt{\frac{\left(2\ell+1\right)\left(2\ell'+1\right)}{4\pi\left(2L+1\right)}}c_{\ell',0,\ell,0}^{L,0}c_{\ell',m',\ell,m}^{L,M}Y_L^M\left(\theta,\varphi\right)\ , \tag{B1}$$

where $c^{L,M}_{\ell',m',\ell,m}$ are the Clebsch–Gordan coefficients [42]. By rewriting trigonometric functions in equation (100) as spherical harmonics,

$$\sin\theta\cos\varphi = \sqrt{\frac{2\pi}{3}}\left(-Y^{l}_{l}(\theta,\varphi)+Y^{1}_{-1}(\theta,\varphi)\right) \tag{B2a}$$

$$\sin\theta\sin\theta = \mathring{\imath}\sqrt{\frac{2\pi}{3}}\left(Y^{l}_{l}(\theta,\varphi)+Y^{1}_{-1}(\theta,\varphi)\right) \tag{B2b}$$

$$\cos\theta = \sqrt{\frac{4\pi}{3}}Y^{0}_{1}(\theta,\varphi)\ , \tag{B2c}$$

and using equation (B1), we arrive at equation (101).

We list the Clebsch–Gordan coefficients of equation (101),

$$c^{L,0}_{1,0,\ell,0} = \delta_{L,\ell+1}\sqrt{\frac{1+\ell}{1+2\ell}} - \delta_{L,\ell-1}\sqrt{\frac{\ell}{1+2\ell}}\,, \tag{B3a}$$

$$c^{L,M}_{1,0,\ell,m} = \delta_{m,M}\left(\delta_{L,\ell+1}\sqrt{\frac{(\ell+1-m)(\ell+1+m)}{(1+\ell)(1+2\ell)}} - \delta_{L,\ell}m\sqrt{\frac{1}{\ell(1+\ell)}} - \delta_{L,\ell-1}\sqrt{\frac{(\ell-m)(\ell+m)}{\ell(2\ell+1)}}\right)\,, \tag{B3b}$$

$$c^{L,M}_{1,1,\ell,m} = \frac{\delta_{m+1,M}}{\sqrt{2}}\left(\delta_{L,\ell+1}\sqrt{\frac{(1+\ell+m)(2+\ell+m)}{(1+\ell)(1+2\ell)}} + \delta_{L,\ell-1}\sqrt{\frac{(\ell-1-m)(\ell-m)}{\ell(1+2\ell)}} + \delta_{L,\ell}\sqrt{\frac{(\ell-m)(1+\ell+m)}{\ell(1+\ell)}}\right)\,, \tag{B3c}$$

$$c^{L,M}_{1,-1,\ell,m} = \frac{\delta_{m-1,M}}{\sqrt{2}}\left(\delta_{L,\ell+1}\sqrt{\frac{(1+\ell-m)(2+\ell-m)}{(1+\ell)(1+2\ell)}} + \delta_{L,\ell-1}\sqrt{\frac{(\ell+m-1)(\ell+m)}{\ell(1+2\ell)}} - \delta_{L,\ell}\sqrt{\frac{(1+\ell-m)(\ell+m)}{\ell(1+\ell)}}\right)\,. \tag{B3d}$$

By substituting the above Clebsch–Gordan coefficients into equation (101), the first two coupling vertices $W^{m',m}_{\ell',\ell}$ on the right hand side of equation (102) are

$$W^{m',m}_{\ell',\ell}(k_x\mathbf{e}_x) = -\mathring{\imath}w_0k_x\sum_{L,M}\sqrt{\frac{2\ell+1}{2(2L+1)}}c^{L,0}_{1,0,\ell,0}\left(-c^{L,M}_{1,1,\ell,m}+c^{L,M}_{1,-1,\ell,m}\right)\delta_{m',M}\delta_{\ell',L} \tag{B4a}$$

$$= -\mathring{\imath}w_0k_x\left\{\frac{\delta_{m',m+1}}{2}\left(-\delta_{\ell',\ell+1}\sqrt{\frac{(1+\ell+m)(2+\ell+m)}{(2\ell+3)(2\ell+1)}} + \delta_{\ell',\ell-1}\sqrt{\frac{(\ell-1-m)(\ell-m)}{(2\ell-1)(2\ell+1)}}\right)\right. \tag{B4b}$$

$$\left. + \frac{\delta_{m',m-1}}{2}\left(\delta_{\ell',\ell+1}\sqrt{\frac{(1+\ell-m)(2+\ell-m)}{(2\ell+3)(2\ell+1)}} - \delta_{\ell',\ell-1}\sqrt{\frac{(\ell+m)(\ell+m-1)}{(2\ell+1)(2\ell-1)}}\right)\right\}, \tag{B4c}$$

$$W^{m',m}_{\ell',\ell}(k_y\mathbf{e}_y) = w_0k_y\sum_{L,M}\sqrt{\frac{2\ell+1}{2(2L+1)}}c^{L,0}_{1,0,\ell,0}\left(c^{L,M}_{1,1,\ell,m}+c^{L,M}_{1,-1,\ell,m}\right)\delta_{m',M}\delta_{\ell',L} \tag{B4d}$$

$$= w_0k_y\left\{\frac{\delta_{m',m+1}}{2}\left(\delta_{\ell',\ell+1}\sqrt{\frac{(1+\ell+m)(2+\ell+m)}{(2\ell+3)(2\ell+1)}} - \delta_{\ell',\ell-1}\sqrt{\frac{(\ell-1-m)(\ell-m)}{(2\ell-1)(2\ell+1)}}\right)\right. \tag{B4e}$$

$$\left. + \frac{\delta_{m',m-1}}{2}\left(\delta_{\ell',\ell+1}\sqrt{\frac{(1+\ell-m)(2+\ell-m)}{(2\ell+3)(2\ell+1)}} - \delta_{\ell',\ell-1}\sqrt{\frac{(\ell+m)(\ell+m-1)}{(2\ell+1)(2\ell-1)}}\right)\right\} \tag{B4f}$$

which together with the third term, $W^{m',m}_{\ell',\ell}(k_z\mathbf{e}_z)$ in equation (103) complete the right hand side of equation (102).

Appendix C. Field Theory of the drift diffusion in an arbitrary potential

In the following we derive the field theory for a drift-diffusion particle in a finite volume with potential $\Upsilon(\mathbf{r})$ and determine the stationary particle density $\rho_0(\mathbf{r})$. Our motivation is two-fold: firstly, we want to reproduce the barometric formula $\rho_0(\mathbf{r}) \propto \exp(-\Upsilon(\mathbf{r})/\mathsf{D}_t)$ in the absence of drift, which is the equilibrium situation of pure diffusion, where the diffusion constant D_t plays the role of the temperature. The barometric formula is Boltzmann's factor, which we want to see reproduced by the field theory as a matter of consistency, section C.4. The derivation will provide us with a template for the more complicated case of a drift. Secondly, we want to determine precisely those corrections due to a constant drift with velocity $\mathbf{w}_0$. We will compare our field-theoretic, perturbative result with the classical calculation in one dimension in section C.5.

We study this phenomenon in a *finite* volume with linear extent L, so that the system develops into a stationary state even in the absence of an external potential, which will be treated perturbatively. In a finite volume, the Fourier series representation of any reasonable (finite, continuous, more generally fulfilling the Dirichlet conditions) potential exists. In an infinite volume, we would have to demand that the potential vanishes at large distances, which may result in the stationary density no longer being normalisable even in the presence of the potential.

To simplify the calculations, we further demand the domain to be periodic. The annihilation field $\chi(\mathbf{r},t)$ and the Doi-shifted creation field $\tilde{\chi}(\mathbf{r},t)$ at position $\mathbf{r}$ and time t can then be written as

$$\tilde{\chi}(\mathbf{r},t) = \frac{1}{L^d}\sum_{\mathbf{n}\in\mathbb{Z}^d}\int_{-\infty}^{\infty} đ\,\omega\, e^{-\mathring{\imath}\omega t} e^{\mathring{\imath}\mathbf{k_n}\cdot\mathbf{r}}\tilde{\chi}(\mathbf{k_n},\omega) \tag{C1a}$$

$$\chi(\mathbf{r},t) = \frac{1}{L^d}\sum_{\mathbf{n}\in\mathbb{Z}^d}\int_{-\infty}^{\infty} đ\,\omega\, e^{-\mathring{\imath}\omega t} e^{\mathring{\imath}\mathbf{k_n}\cdot\mathbf{r}}\chi(\mathbf{k_n},\omega) \tag{C1b}$$

with the notation in keeping with the rest of the present work. The finite volume we have chosen to be a cube with linear extension L, easily generalisable to a cuboid or similar. The Fourier modes are $\mathbf{k_n} = 2\pi\mathbf{n}/L$ with $\mathbf{n} = (n_1, n_2, \ldots, n_d)^\mathsf{T}$ a d-dimensional integer in $\mathbb{Z}^d$. We further use the notation $đ = \mathrm{d}/(2\pi)$ and later, correspondingly, $\delta\!\!\!{}^-(\omega) = 2\pi\delta(\omega)$ to cancel that factor of 2π.

The time-independent potential $\Upsilon(\mathbf{r})$ follows the convention equation (32), restated here for convenience in arbitrary dimensions

$$\Upsilon(\mathbf{r}) = \frac{1}{L^d}\sum_{\mathbf{n}\in\mathbb{Z}^d}\Upsilon_\mathbf{n} e^{\mathring{\imath}\mathbf{k_n}\cdot\mathbf{r}} \tag{C2a}$$

$$\Upsilon_\mathbf{n} = \int_0^L \ldots \int_0^L \mathrm{d}^d r\, \Upsilon(\mathbf{r})\, e^{-\mathring{\imath}\mathbf{k_n}\cdot\mathbf{r}}\,. \tag{C2b}$$

C.1. Action

The Fokker–Planck equation of the fully time-dependent density $\rho(\mathbf{r},t)$ of particles at position $\mathbf{r}$ and time t, subject to diffusion with constant D_t and drift with velocity $\mathbf{w}$, in a potential $\Upsilon(\mathbf{r})$ can be written as

$$\partial_t\rho(\mathbf{r},t) = \mathsf{D}_t\nabla_\mathbf{r}^2\rho(\mathbf{r},t) - \nabla_\mathbf{r}\cdot(\rho(\mathbf{r},t)(\mathbf{w} - \nabla\Upsilon(\mathbf{r}))) \tag{C3}$$

removing all ambiguity about the action of the gradient operators by stating that they act on all objects to their right.

The action of particles with diffusion constant D_t and moving ballistically with velocity $\mathbf{w}_0$ is [11]

$$\mathcal{A}_0[\tilde{\chi},\chi] = -\int đ\,\omega\,\frac{1}{L^d}\sum_{\mathbf{n}\in\mathbb{Z}^d}\tilde{\chi}(-\mathbf{k_n},-\omega)\chi(\mathbf{k_n},\omega)\left(-\mathring{\imath}\omega + \mathsf{D}_t k_\mathbf{n}^2 + \mathring{\imath}\mathbf{w}_0\cdot\mathbf{k_n} + m\right) \tag{C4}$$

with $k_\mathbf{n} = |\mathbf{k_n}|$ and $m \downarrow 0$ a mass to regularise the infrared and establish causality. An additional external potential results in an additional space-dependent drift term and thus in the action

$$\mathcal{A}_P = \int \mathrm{d}^d r \int \mathrm{d}t\, \tilde{\chi}(\mathbf{r},t)\nabla_\mathbf{r}\cdot(\nabla_\mathbf{r}\Upsilon(\mathbf{r}))\chi(\mathbf{r},t) \tag{C5a}$$

$$= \int đ\,\omega\,\frac{1}{L^{3d}}\sum_{\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3}\mathbf{k}_{\mathbf{n}_1}\cdot\mathbf{k}_{\mathbf{n}_2}\tilde{\chi}(\mathbf{k}_{\mathbf{n}_1},-\omega)\Upsilon_{\mathbf{n}_2}\chi(\mathbf{k}_{\mathbf{n}_3},\omega)L^d\delta_{\mathbf{n}_1+\mathbf{n}_2+\mathbf{n}_3,\mathbf{0}} \tag{C5b}$$

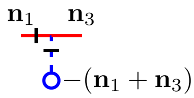
e.g. equations (9b) or (31a) to be treated perturbatively, equation (8).

The bare propagator follows immediately from equation (C4),

$$\langle \chi(\mathbf{k_n},\omega)\tilde{\chi}(\mathbf{k_p},\omega_0)\rangle_0 = \frac{\delta\!\!\!^-(\omega+\omega_0)L^d\delta_{\mathbf{n+p,0}}}{-\imath\omega + \mathrm{D}_t k_{\mathbf{n}}^2 + \imath\mathbf{w}_0\cdot\mathbf{k} + m} = \delta\!\!\!^-(\omega+\omega_0)L^d\delta_{\mathbf{n+p,0}}G(\mathbf{k_n},\omega) \triangleq \tag{C6}$$

and the perturbative part of the action provides a single vertex with a 'bauble'

$$\mathbf{k_{n_1}}\cdot\mathbf{k}_{-(\mathbf{n_1+n_3})}\Upsilon_{-(\mathbf{n_1+n_3})} \triangleq \tag{C7}$$



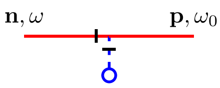
to be summed over.

C.2. Propagator

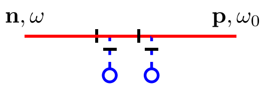
With the help of equations (C6) and (C7) the full propagator can be written perturbatively,

$$\langle \chi(\mathbf{k_n},\omega)\tilde{\chi}(\mathbf{k_p},\omega_0)\rangle \triangleq \tag{C8}$$

$+$



$+$



$+\ldots$

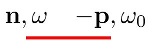
$$= \delta\!\!\!^-\;(\omega+\omega_0)\left\{L^d\delta_{\mathbf{n+p},0}G(\mathbf{k_n},\omega) + G(\mathbf{k_n},\omega)\mathbf{k_{-n}}\cdot\mathbf{k_{n+p}}\Upsilon_{\mathbf{n+p}}G(-\mathbf{k_p},\omega)+\ldots\right\}. \tag{C9}$$

More systematically, the full propagator may be expanded as

$$\left\langle \chi(\mathbf{k_n},\omega)\,\tilde{\chi}(-\mathbf{k_p},\omega_0)\right\rangle = \delta\!\!\!^-\;(\omega+\omega_0)\sum_{j=0}^{\infty} E_j(\mathbf{k_n},\mathbf{k_p},\omega) \tag{C10}$$

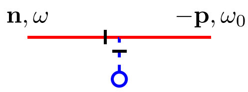
where we changed the sign of $\mathbf{k_p}$ in the creator field compared to equation (C8) to improve notation below. The expansion terms E_j are defined as follows

$$E_0(\mathbf{k_n},\mathbf{k_p},\omega) = L^d\delta_{\mathbf{n-p},0}G(\mathbf{k_n},\omega) \tag{C11a}$$

$\triangleq$ 

,

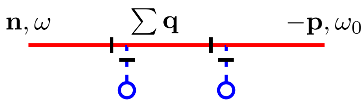
$$E_1(\mathbf{k_n},\mathbf{k_p},\omega) = -G(\mathbf{k_n},\omega)\,\mathbf{k_n}\cdot\mathbf{k_{n-p}}\Upsilon_{\mathbf{n-p}}G(\mathbf{k_p},\omega \tag{C11b}$$

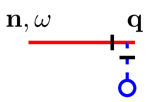
$\triangleq$ 

,

$$E_2(\mathbf{k_n},\mathbf{k_p},\omega) = G(\mathbf{k_n},\omega)\frac{1}{L^d}\sum_{\mathbf{q}\in\mathbb{Z}^d}(\mathbf{k_n}\cdot\mathbf{k_{n-q}})\Upsilon_{\mathbf{n-q}}G(\mathbf{k_q},\omega)\,(\mathbf{k_q}\cdot\mathbf{k_{q-p}})\Upsilon_{\mathbf{q-p}}G(\mathbf{k_p},\omega)$$

$$= -G(\mathbf{k_n},\omega)\frac{1}{L^d}\sum_{\mathbf{q}\in\mathbb{Z}^d}(\mathbf{k_n}\cdot\mathbf{k_{n-q}})\Upsilon_{\mathbf{n-q}}E_1(\mathbf{k_q},\mathbf{k_p},\omega) \tag{C11c}$$

$\triangleq$ 

$= \frac{1}{L^d}\sum_{\mathbf{q}\in\mathbb{Z}^d}$ 

$E_1(\mathbf{k_q},\mathbf{k_p},\omega),$

with the general recurrence

$$E_{j+1}(\mathbf{k_n},\mathbf{k_p},\omega) = -G(\mathbf{k_n},\omega)\frac{1}{L^d}\sum_{\mathbf{q}\in\mathbb{Z}^d}(\mathbf{k_n}\cdot\mathbf{k_{n-q}})\Upsilon_{\mathbf{n-q}}E_j(\mathbf{k_q},\mathbf{k_p},\omega) \tag{C12}$$

amounting to a convolution to be analysed further below.

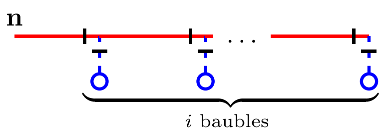
C.3. Stationary state

The density $\rho_0(\mathbf{r})$ in the stationary or steady state is found by taking of the propagator the limit $t_0 \to -\infty$ of the time of the initial deposition,

$$\rho_0(\mathbf{r}) = \lim_{t_0 \to -\infty} \langle \chi(\mathbf{r}, t) \tilde{\chi}(\mathbf{r}_0, t_0) \rangle \tag{C13}$$

expected to be independent of $\mathbf{r}_0$ and t, provided the system is ergodic and possesses a (unique) stationary state. Provided all internal legs are dashed, i.e. they carry a factor $\mathbf{k}$, the diagrammatic mechanics of this limit amounts to an amputation of the incoming leg in any composite diagram. This is most easily understood by taking the inverse Fourier transform from ω, ω_0 to t, t_0, while leaving the spatial dependence in $\mathbf{k}$, starting from the propagators that have the form equation (C6). The inverse Fourier transform will result in exponentials of the form $\mathrm{e}^{-\mathring{\imath} t_0 s}$, where s is the location of the pole of the propagators, here $s = \mathring{\imath}(\mathsf{D}_t k_{\mathbf{n}}^2 + \mathring{\imath}\mathbf{w}_0 \cdot \mathbf{k}_{\mathbf{n}} + m)$ with $\Im(s) \geqslant 0$. Only if the imaginary part of s vanishes, the exponential will not vanish as $t_0 \to -\infty$. This happens only when $\mathbf{n} = \mathbf{0}$ and in the limit of $m \downarrow 0$. The resulting residue is thus determined by the remainder of the diagram evaluated at the pole $\omega = 0$ and with the incoming leg replaced by $\delta_{\mathbf{p},\mathbf{0}}$, so that an inverse Fourier transform in $\mathbf{k}_{\mathbf{p}}$ to $\mathbf{r}_0$ results in a factor $1/L^d$. As for the individual propagator equation (C11a) in equation (C10), it contributes indeed only this background, $1/L^d$. Writing therefore E_i with only one argument as the desired limit,

$$E_i(\mathbf{k}_{\mathbf{n}}) = \lim_{t_0 \to -\infty} \lim_{m \downarrow 0} \int đ\omega_0\, \mathrm{e}^{-\mathring{\imath}\omega_0 (t_0 - t)} \frac{1}{L^d} \sum_{\mathbf{p} \in \mathbb{Z}} \mathrm{e}^{\mathring{\imath}\mathbf{k}_{\mathbf{p}} \cdot \mathbf{r}_0} E_i(\mathbf{k}_{\mathbf{n}}, \mathbf{k}_{\mathbf{p}}, -\omega_0) \tag{C14}$$

$\triangleq$ 

allows the stationary density to be written in the form

$$\rho_0(\mathbf{r}) = \frac{1}{L^d} \sum_{\mathbf{n} \in \mathbb{Z}} \mathrm{e}^{\mathring{\imath}\mathbf{k}_{\mathbf{n}} \cdot \mathbf{r}} \sum_{j=0}^{\infty} E_j(\mathbf{k}_{\mathbf{n}}) \tag{C15}$$

via equations (C10) and (C13) and gives

$$E_0(\mathbf{k}_{\mathbf{n}}) = L^d \delta_{\mathbf{n},\mathbf{0}} \frac{1}{L^d} = \delta_{\mathbf{n},\mathbf{0}} \tag{C16}$$

from equation (C11a) and

$$E_1(\mathbf{k}_{\mathbf{n}}) = -G(\mathbf{k}_{\mathbf{n}}, 0)\, \mathbf{k}_{\mathbf{n}} \cdot \mathbf{k}_{\mathbf{n}} \mathcal{I}(\mathbf{n} \neq \mathbf{0})\, \Upsilon_{\mathbf{n}} \frac{1}{L^d} = -\frac{1}{L^d} \frac{k_{\mathbf{n}}^2 \Upsilon_{\mathbf{n}} \mathcal{I}(\mathbf{n} \neq \mathbf{0})}{\mathsf{D}_t k_{\mathbf{n}}^2 + \mathring{\imath}\mathbf{w}_0 \cdot \mathbf{k}_{\mathbf{n}}}, \tag{C17}$$

using equation (C6) and where

$$\mathcal{I}(\mathbf{n} \neq \mathbf{0}) = 1 - \delta_{\mathbf{n},\mathbf{0}} \tag{C18}$$

accounts for the subtlety that the right hand side of equation (C11b) strictly vanishes for $\mathbf{n} = \mathbf{0}$, because of the $\mathbf{k}_{\mathbf{n}}$ prefactor and all other terms being finite as $m \neq 0$. However, in equation (C14) the limit $m \downarrow 0$ has to be taken so that $t_0 \to -\infty$ produces a finite result, resulting in

$$\lim_{m \downarrow 0} \frac{\mathbf{k}_{\mathbf{n}}}{\mathbf{k}_{\mathbf{n}}^2 + m} = \frac{\mathbf{k}_{\mathbf{n}}}{\mathbf{k}_{\mathbf{n}}^2} \mathcal{I}(\mathbf{n} \neq \mathbf{0}) = \begin{cases} \mathbf{0} & \text{for } \mathbf{k} = \mathbf{0} \\ \mathbf{k}_{\mathbf{n}}/\mathbf{k}_{\mathbf{n}}^2 & \text{otherwise}, \end{cases} \tag{C19}$$

using the convention $0\infty = 0$. The indicator function equation (C18) needs to be in place for every prefactor $\mathbf{k}$ that also features in the denominator of a propagator $G(\mathbf{k}, 0)$ so that the limits $m \downarrow 0$ and $t \to \infty$ can safely be taken.

For easier comparison, we state the expansion of the density to first order in the potential for drift-diffusion particles in a finite volume determined explicitly so far,

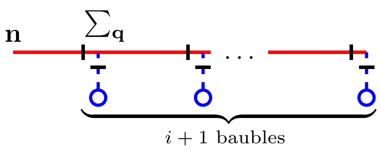
$$\rho_0(\mathbf{r}) = \frac{1}{L^d} - \frac{1}{L^{2d}} \sum_{\substack{\mathbf{n}\in\mathbb{Z} \\ \mathbf{n}\neq\mathbf{0}}} \mathrm{e}^{\mathring{\imath}\mathbf{k}_\mathbf{n}\cdot\mathbf{r}} \frac{k_\mathbf{n}^2 \Upsilon_\mathbf{n}}{\mathsf{D}_t k_\mathbf{n}^2 + \mathring{\imath}\mathbf{w}_0\cdot\mathbf{k}_\mathbf{n}} + \dots \tag{C20}$$

using equations (C15)–(C17).

With the indicator function equation (C18) suppressing unwanted singularities, the recurrence equation (C12) remains essentially unchanged at stationary, as only the outgoing propagator needs to be adjusted to $\omega = 0$,

$$E_{j+1}(\mathbf{k}_\mathbf{n}) = -G(\mathbf{k}_\mathbf{n}, 0)\frac{1}{L^d}\sum_{\mathbf{q}\in\mathbb{Z}^d} \mathcal{I}(\mathbf{n}\neq\mathbf{0})(\mathbf{k}_\mathbf{n}\cdot\mathbf{k}_{\mathbf{n}-\mathbf{q}})\Upsilon_{\mathbf{n}-\mathbf{q}}E_j(\mathbf{k}_\mathbf{q}) \tag{C21a}$$

$$= -\frac{\mathcal{I}(\mathbf{n}\neq\mathbf{0})}{\mathsf{D}_t k_\mathbf{n}^2 + \mathring{\imath}\mathbf{w}_0\cdot\mathbf{k}_\mathbf{n}}\frac{1}{L^d}\sum_{\mathbf{q}\in\mathbb{Z}^d}(\mathbf{k}_\mathbf{n}\cdot\mathbf{k}_{\mathbf{n}-\mathbf{q}})\Upsilon_{\mathbf{n}-\mathbf{q}}E_j(\mathbf{k}_\mathbf{q}) \tag{C21b}$$

$\triangleq$ 

(C21c)

using equation (C6). In one dimension we can further simplify,

$$E_{j+1}(k_n) = -\frac{\mathcal{I}(n\neq 0)}{\mathsf{D}_t k_n + \mathring{\imath}w_0}\frac{1}{L}\sum_{q\in\mathbb{Z}}\Upsilon_{n-q}k_{n-q}E_j(k_q) \ . \tag{C22}$$

From equation (C21) it can be gleaned that in real-space $E_j(\mathbf{r})$ obeys the recurrence

$$\left(\mathsf{D}_t\nabla_\mathbf{r}^2 - \mathbf{w}\cdot\nabla_\mathbf{r}\right)E_{j+1}(\mathbf{r}) = -\nabla_\mathbf{r}\left(E_j(\mathbf{r})\nabla_\mathbf{r}\Upsilon(\mathbf{r})\right) \ , \tag{C23}$$

where we have refrained from introducing a separate symbol for the inverse Fourier transform $E_j(\mathbf{r})$ of $E_j(\mathbf{k})$. It is instructive to demonstrate that this implies that equation (C15) therefore solves the Fokker-Planck equation (C3) at stationarity, i.e. we want to show that using equation (C23) in equation (C15) provides a solution of equation (C3) with $\partial_t\rho = 0$,

$$0 = \mathsf{D}_t\nabla_\mathbf{r}^2\rho_0(\mathbf{r}) - \nabla_\mathbf{r}\cdot(\rho_0(\mathbf{r})(\mathbf{w} - \nabla\Upsilon(\mathbf{r}))) \ . \tag{C24}$$

To see this, we sum both sides of equation (C23) over $j = 0\dots$, which on the left-hand side produces ρ_0 of equation (C15), including the vanishing term

$$\left(\mathsf{D}_t\nabla_\mathbf{r}^2 - \mathbf{w}\cdot\nabla_\mathbf{r}\right)E_0(\mathbf{r}) = 0 \tag{C25}$$

as $E_0(\mathbf{r}) = L^{-d}$, equation (C16), so that equation (C23) implies

$$\left(\mathsf{D}_t\nabla_\mathbf{r}^2 - \mathbf{w}\cdot\nabla_\mathbf{r}\right)\sum_{j=0}^{\infty}E_j(\mathbf{r}) = -\nabla_\mathbf{r}\left(\sum_{j=0}^{\infty}E_j(\mathbf{r})\nabla_\mathbf{r}\Upsilon(\mathbf{r})\right) \ , \tag{C26}$$

and thus equation (C24), with the E_j in equation (C15) determined by equation (C21).

Equation (C21) is the central result of the present section. By means of equation (C15), it allows the calculation of the stationary density starting from E_0, equation (C16). Without drift, the density should produce the Boltzmann factor, which we will recover in the next section. While this result is easy to obtain from a differential equation approach in real-space $\mathbf{r}$, it is very instructive to perform this calculation in $\mathbf{k}$-space. With drift, on the other hand, we can compare the density ρ_0 resulting from equation (C21) to the known stationary density in one dimension [53], which is done in section C.5.

C.4. Barometric formula

In the absence of a drift, $\mathbf{w} = \mathbf{0}$, the density will evolve into the Boltzmann factor

$$\rho_0(\mathbf{r}) = \frac{1}{\mathcal{N}} \mathrm{e}^{-\Upsilon(\mathbf{r})/\mathsf{D}_t} \tag{C27}$$

with normalisation constant

$$\mathcal{N} = \int \mathrm{d}^d r \, \mathrm{e}^{-\Upsilon(\mathbf{r})/\mathsf{D}_t} . \tag{C28}$$

Equation (C27) is the stationary solution of the Fokker-Planck equation (C3) without drift,

$$0 = \mathsf{D}_t \nabla^2_{\mathbf{r}} \rho_0(\mathbf{r}) + \nabla_{\mathbf{r}} \left(\rho_0(\mathbf{r}) \nabla_{\mathbf{r}} \Upsilon(\mathbf{r}) \right) , \tag{C29}$$

which demands that the probability current is spatially uniform [54]. Provided the potential is bounded from above and from below and with boundary conditions given, the solution is unique by equation (C27), including the normalisation constant given by equation (C28).

In the following, we show the equivalence of equation (C27) and the field-theoretic result equations (C15), (C16) and (C21), by expanding the density ρ_0 from equation (C27) in terms of some B_j, to be characterised next.

C.4.1. Properties of $B_j(\mathbf{k_n})$

We expand the exponential in equation (C27) order by order in the potential

$$\rho_0(\mathbf{r}) = \mathcal{N}^{-1} \sum_{j=0}^{\infty} \frac{1}{j!} \left(-\frac{\Upsilon(\mathbf{r})}{\mathsf{D}_t} \right)^j \tag{C30}$$

and introduce Fourier-modes

$$B_j(\mathbf{k_n}) = \int_0^L \dots \int_0^L \mathrm{d}^d r \, \mathrm{e}^{-\imath \mathbf{k_n} \cdot \mathbf{r}} \frac{1}{j!} \left(-\frac{\Upsilon(\mathbf{r})}{\mathsf{D}_t} \right)^j \tag{C31}$$

so that

$$\rho_0(\mathbf{r}) = \mathcal{N}^{-1} \sum_{j=0}^{\infty} \frac{1}{L^d} \sum_{\mathbf{n} \in \mathbb{Z}} \mathrm{e}^{\imath \mathbf{k_n} \cdot \mathbf{r}} B_j(\mathbf{k_n}) , \tag{C32}$$

similar to equation (C15). The normalisation equation (C28) can therefore be written as a sum over the $\mathbf{0}$-modes of B_j in equation (C31)

$$\mathcal{N} = \sum_{j=0}^{\infty} B_j(\mathbf{0}) . \tag{C33}$$

That $E_j(\mathbf{r})$ as used in equation (C15) and defined in equation (C14) solves equation (C29) has been established in equation (C26) via the recurrence equation (C21). By construction, the E_j, in equation (C15) provide an expansion of the density order by order in the potential Υ. The B_j, equation (C32), on the other hand, are an expansion in orders of the potential of only the exponential, lacking, however, the normalisation. Both E_j and B_j are, by construction, of order j in the potential Υ. While generally $E_j(\mathbf{k_n}) \neq B_j(\mathbf{k_n})/\mathcal{N}$, we will show in the following that

$$\rho_0(\mathbf{k_n}) = \sum_{j=0}^{\infty} E_j(\mathbf{k_n}) = \frac{\sum_{j=0}^{\infty} B_j(\mathbf{k_n})}{B_0(\mathbf{0}) + B_1(\mathbf{0}) + \dots} , \tag{C34}$$

taking the Fourier transform on both sides of equations (C15) and (C32), and using equation (C33). Equivalently, we show that $B_j(\mathbf{k_n})$ is the sum of the terms of jth order in Υ of $\mathcal{N} \sum_j E_j(\mathbf{k_n})$,

$$\sum_{i=0}^{j} B_i(\mathbf{0}) E_{j-i}(\mathbf{k_n}) = B_j(\mathbf{k_n}) . \tag{C35}$$

We will thus show, beyond equation (C26), that the E_j are correctly normalised, providing us with an expansion of the density ρ_0 order by order in the potential. Showing this, will further provide us with a useful, non-trivial algebraic identity.

To proceed, we firstly confirm equation (C35) for $j=0,1$ by determining $B_j(\mathbf{k})$ directly from equation (C31)

$$B_0\left(\mathbf{k}_\mathbf{n}\right) = L^d \delta_{\mathbf{n},\mathbf{0}} \tag{C36a}$$

$$B_1\left(\mathbf{k}_\mathbf{n}\right) = -\frac{\Upsilon_\mathbf{n}}{\mathsf{D}_t} \tag{C36b}$$

so that equation (C16) indeed confirms

$$B_0\left(\mathbf{0}\right) E_0\left(\mathbf{k}_\mathbf{n}\right) = L^d \delta_{\mathbf{n},\mathbf{0}} = B_0\left(\mathbf{k}_\mathbf{n}\right) \tag{C37}$$

and equations (C16) and (C17) with $\mathbf{w}=\mathbf{0}$ confirm

$$B_0\left(\mathbf{0}\right) E_1\left(\mathbf{k}_\mathbf{n}\right) + B_1\left(\mathbf{0}\right) E_0\left(\mathbf{k}_\mathbf{n}\right) = -L^d \frac{\Upsilon_\mathbf{n}\mathcal{I}\left(\mathbf{n}\neq\mathbf{0}\right)}{\mathsf{D}_t}\frac{1}{L^d} - \frac{\Upsilon_\mathbf{0}}{\mathsf{D}_t}\delta_{\mathbf{n},\mathbf{0}} = -\frac{\Upsilon_\mathbf{n}}{\mathsf{D}_t}\left(\mathcal{I}\left(\mathbf{n}\neq\mathbf{0}\right) + \delta_{\mathbf{n},\mathbf{0}}\right) = B_1\left(\mathbf{k}_\mathbf{n}\right) \tag{C38}$$

as $\Upsilon_\mathbf{0}\delta_{\mathbf{n},\mathbf{0}} = \Upsilon_\mathbf{n}\delta_{\mathbf{n},\mathbf{0}}$ and

$$1 = \mathcal{I}\left(\mathbf{n}\neq\mathbf{0}\right) + \delta_{\mathbf{n},\mathbf{0}} . \tag{C39}$$

To characterise B_j more generally, we introduce the recursion formula

$$B_{j+1}\left(\mathbf{k}_\mathbf{n}\right) = -\frac{1}{\left(j+1\right)\mathsf{D}_t}\frac{1}{L^d}\sum_{\mathbf{q}\in\mathbb{Z}^d}\Upsilon_{\mathbf{n}-\mathbf{q}}B_j\left(\mathbf{k}_\mathbf{q}\right) \tag{C40}$$

by elementary calculations on the basis of equation (C31) and similar to equation (C21). Starting from equation (C36a), it can be used to produce for $j\geqslant 2$

$$B_j\left(\mathbf{k}_\mathbf{n}\right) = \frac{L^d}{j!}\left(\frac{-1}{L^d\mathsf{D}_t}\right)^j \sum_{\mathbf{n}_{j-1},\ldots,\mathbf{n}_1} \underbrace{\Upsilon_{\mathbf{n}-\mathbf{n}_{j-1}}\Upsilon_{\mathbf{n}_{j-1}-\mathbf{n}_{j-2}}\ldots\Upsilon_{\mathbf{n}_2-\mathbf{n}_1}\Upsilon_{\mathbf{n}_1}}_{j\text{ factors of }\Upsilon} . \tag{C41}$$

This expression can be simplified further by substituting dummy variables according to $\mathbf{p}_i = \mathbf{n}_i - \mathbf{n}_{i-1}$ for $i = j-1, j-2, \ldots, 1$ with the convention $\mathbf{n}_0 = \mathbf{0}$. As for

$$\mathbf{p}_j = \mathbf{n} - \mathbf{n}_{j-1} = \mathbf{n} - \mathbf{p}_{j-1} - \mathbf{n}_{j-2} = \ldots = \mathbf{n} - \mathbf{p}_{j-1} - \mathbf{p}_{j-2} - \ldots - \mathbf{p}_1 , \tag{C42}$$

this can be allowed to run in the sum by enforcing equation (C42) via a Kronecker δ-function, so that eventually

$$B_j\left(\mathbf{k}_\mathbf{n}\right) = \frac{L^d}{j!}\left(\frac{-1}{L^d\mathsf{D}_t}\right)^j \sum_{\mathbf{p}_j,\ldots,\mathbf{p}_1} \Upsilon_{\mathbf{p}_j}\Upsilon_{\mathbf{p}_{j-1}}\ldots\Upsilon_{\mathbf{p}_1}\delta_{\mathbf{p}_1+\ldots+\mathbf{p}_j,\mathbf{n}} . \tag{C43}$$

Even when calculated with a convolution in mind, equation (C43) is valid for $j=1$ by direct comparison with equation (C36b) and, by comparison with equation (C36a), even $j=0$ with the convention that the final $\delta_{\mathbf{p}_1+\ldots+\mathbf{p}_j,\mathbf{n}}$ degenerates into $\delta_{\mathbf{0},\mathbf{n}}$ for $j=0$.

In the form equation (C43), we can show easily an important identity, based on the observation

$$\sum_{\mathbf{p}_j,\ldots,\mathbf{p}_1} \mathbf{k}_{\mathbf{p}_j}\Upsilon_{\mathbf{p}_j}\Upsilon_{\mathbf{p}_{j-1}}\ldots\Upsilon_{\mathbf{p}_1}\delta_{\mathbf{p}_1+\ldots\mathbf{p}_j,\mathbf{n}} = \sum_{\mathbf{p}_j,\ldots,\mathbf{p}_1} \mathbf{k}_{\mathbf{p}_i}\Upsilon_{\mathbf{p}_j}\Upsilon_{\mathbf{p}_{j-1}}\ldots\Upsilon_{\mathbf{p}_1}\delta_{\mathbf{p}_1+\ldots\mathbf{p}_j,\mathbf{n}} \tag{C44}$$

for all $i\in\{1,2,\ldots,j\}$, which labels the index of $\mathbf{k}_{\mathbf{p}_i}$ on the right-hand side as the $\mathbf{p}_i$ are all equivalent dummy variables. Summing this sum for $i=1,2,\ldots,j$ therefore gives j times the same result, while the sum of the $\mathbf{k}_{\mathbf{p}_i}$ gives $\mathbf{k}_{\mathbf{p}_1}+\ldots+\mathbf{k}_{\mathbf{p}_j} = \mathbf{k}_\mathbf{n}$ inside the sum, according to the Kronecker δ-function. In conclusion for $j\geqslant 1$

$$j\sum_{\mathbf{p}_j,\ldots,\mathbf{p}_1} \mathbf{k}_{\mathbf{p}_j}\Upsilon_{\mathbf{p}_j}\Upsilon_{\mathbf{p}_{j-1}}\ldots\Upsilon_{\mathbf{p}_1}\delta_{\mathbf{p}_1+\ldots\mathbf{p}_j,\mathbf{n}} = \mathbf{k}_\mathbf{n}\sum_{\mathbf{p}_j,\ldots,\mathbf{p}_1} \Upsilon_{\mathbf{p}_j}\Upsilon_{\mathbf{p}_{j-1}}\ldots\Upsilon_{\mathbf{p}_1}\delta_{\mathbf{p}_1+\ldots\mathbf{p}_j,\mathbf{n}} , \tag{C45}$$

and thus

$$\sum_{\mathbf{p}_j,\dots,\mathbf{p}_1} \mathcal{I}(\mathbf{n}\neq\mathbf{0}) \frac{\mathbf{k}_\mathbf{n}\cdot\mathbf{k}_{\mathbf{p}_j}}{k_\mathbf{n}^2} \Upsilon_{\mathbf{p}_j}\Upsilon_{\mathbf{p}_{j-1}}\dots\Upsilon_{\mathbf{p}_1}\delta_{\mathbf{p}_1+\dots\mathbf{p}_j,\mathbf{n}} = \frac{1}{j}\sum_{\mathbf{p}_j,\dots,\mathbf{p}_1} \Upsilon_{\mathbf{p}_j}\Upsilon_{\mathbf{p}_{j-1}}\dots\Upsilon_{\mathbf{p}_1}\delta_{\mathbf{p}_1+\dots\mathbf{p}_j,\mathbf{n}}\,, \tag{C46}$$

where the indicator function on the left avoids the divergence of $\mathbf{k}_\mathbf{n}\cdot\mathbf{k}_{\mathbf{p}_j}/k_\mathbf{n}^2$. Using equation (C46) in equation (C43) gives

$$\mathcal{I}(\mathbf{n}\neq\mathbf{0})B_j(\mathbf{k}_\mathbf{n}) = \mathcal{I}(\mathbf{n}\neq\mathbf{0})\frac{L^d}{(j-1)!}\left(\frac{-1}{L^d\mathsf{D}_t}\right)^j \sum_{\mathbf{p}_j,\dots,\mathbf{p}_1}\frac{\mathbf{k}_\mathbf{n}\cdot\mathbf{k}_{\mathbf{p}_j}}{k_\mathbf{n}^2}\Upsilon_{\mathbf{p}_j}\Upsilon_{\mathbf{p}_{j-1}}\dots\Upsilon_{\mathbf{p}_1}\delta_{\mathbf{p}_1+\dots\mathbf{p}_j,\mathbf{n}} \tag{C47a}$$

$$= \mathcal{I}(\mathbf{n}\neq\mathbf{0})\frac{L^d}{(j-1)!}\left(\frac{-1}{L^d\mathsf{D}_t}\right)^j \sum_{\mathbf{n}_{j-1},\dots,\mathbf{n}_1}\frac{\mathbf{k}_\mathbf{n}\cdot\mathbf{k}_{\mathbf{n}-\mathbf{n}_{j-1}}}{k_\mathbf{n}^2}\Upsilon_{\mathbf{n}-\mathbf{n}_{j-1}}\Upsilon_{\mathbf{n}_{j-1}-\mathbf{n}_{j-2}}\dots\Upsilon_{\mathbf{n}_2-\mathbf{n}_1}\Upsilon_{\mathbf{n}_1} \tag{C47b}$$

$$= -\frac{\mathcal{I}(\mathbf{n}\neq\mathbf{0})}{\mathsf{D}_t}\frac{1}{L^d}\sum_{\mathbf{n}_{j-1}\in\mathbb{Z}^d}\frac{\mathbf{k}_\mathbf{n}\cdot\mathbf{k}_{\mathbf{n}-\mathbf{n}_{j-1}}}{k_\mathbf{n}^2}\Upsilon_{\mathbf{n}-\mathbf{n}_{j-1}}B_{j-1}\left(\mathbf{k}_{\mathbf{n}_{j-1}}\right) \tag{C47c}$$

where the second equality is a matter of labelling the indices again in $\mathbf{n}$ and $\mathbf{n}_{1\dots j-1}$ using equation (C42) in reverse, and thus reverting from the indexing in equation (C43) to that in equation (C41), which does not carry a Kronecker δ-function. In this form the summation can again be written recursively, similarly to equation (C40), which is done after the third equality, by absorbing the summation over $\mathbf{n}_{j-2},\dots,\mathbf{n}_1$ into $B_{j-1}(\mathbf{k}_{\mathbf{n}_{j-1}})$. Equation (C47*c*) is the key outcome of the present section.

C.4.2. Relationship between $E_j(\mathbf{k}_\mathbf{n})$ and $B_j(\mathbf{k}_\mathbf{n})$

We proceed with confirming equation (C35) by induction, using equation (C47*c*) in the course. To access this identity, we firstly rewrite equation (C35) using equation (C39), so that for $j\geqslant 0$

$$B_{j+1}(\mathbf{k}_\mathbf{n}) = B_{j+1}(\mathbf{k}_\mathbf{n})\left(\mathcal{I}(\mathbf{n}\neq\mathbf{0})+\delta_{\mathbf{n},\mathbf{0}}\right) = -\frac{\mathcal{I}(\mathbf{n}\neq\mathbf{0})}{\mathsf{D}_t}\frac{1}{L^d}\sum_{\mathbf{n}_j\in\mathbb{Z}^d}\frac{\mathbf{k}_\mathbf{n}\cdot\mathbf{k}_{\mathbf{n}-\mathbf{n}_j}}{k_\mathbf{n}^2}\Upsilon_{\mathbf{n}-\mathbf{n}_j}B_j\left(\mathbf{k}_{\mathbf{n}_j}\right) + B_{j+1}(\mathbf{k}_\mathbf{n})\delta_{\mathbf{n},\mathbf{0}}\,. \tag{C48}$$

Of the two terms on the right hand side, the first can be rewritten using equation (C35), which is *assumed* to hold for j. This allows us to replace $B_j(\mathbf{k}_{\mathbf{n}_j})$ by a sum. In the second term we replace $\delta_{\mathbf{n},\mathbf{0}}$ by $E_0(\mathbf{k}_n)$ according to equation (C16), resulting in

$$B_{j+1}(\mathbf{k}_\mathbf{n}) = -\frac{\mathcal{I}(\mathbf{n}\neq\mathbf{0})}{\mathsf{D}_t}\frac{1}{L^d}\sum_{\mathbf{n}_j\in\mathbb{Z}^d}\frac{\mathbf{k}_\mathbf{n}\cdot\mathbf{k}_{\mathbf{n}-\mathbf{n}_j}}{k_\mathbf{n}^2}\Upsilon_{\mathbf{n}-\mathbf{n}_j}\sum_{i=0}^{j}B_i(\mathbf{0})E_{j-i}\left(\mathbf{k}_{\mathbf{n}_j}\right) + B_{j+1}(\mathbf{0})E_0(\mathbf{k}_n)\,. \tag{C49}$$

The summation over $\mathbf{n}_j\in\mathbb{Z}^d$ can now be performed on E_{j-i} using equation (C21) at $\mathbf{w}=\mathbf{0}$,

$$B_{j+1}(\mathbf{k}_\mathbf{n}) = \sum_{i=0}^{j}B_i(\mathbf{0})E_{j-i+1}(\mathbf{k}_\mathbf{n}) + B_{j+1}(\mathbf{0})E_0(\mathbf{k}_n) = \sum_{i=0}^{j+1}B_i(\mathbf{0})E_{j+1-i}(\mathbf{k}_\mathbf{n}) \quad \text{for } j\geqslant 0\,, \tag{C50}$$

completing our demonstration that equation (C35) holds for $j+1$ if it holds for j. With the induction basis equation (C37) or (C38) this concludes our demonstration that the diagrams equation (C14) or equivalently (C21) produce a normalised expansion of the density ρ_0 (C15) identical to the Boltzmann factor, order by order in the external potential. The field-theoretic approach thus determines the stationary density without the need of an *a posteriori* normalisation. And while the field theory is an expansion necessarily in a sufficiently weak potential and necessarily in a finite volume, no such restriction applies to the resulting Boltzmann factor.

In the next section we will similarly demonstrate the correspondence between classical and field-theoretic stationary density in the presence of a drift w.

C.5. Density in one dimension with drift

In this section, we will demonstrate that the expansion equation (C15) in terms of diagrams equation (C14) produces the correct, normalised, stationary result in the presence of a potential and a drift in one dimension. The restriction to one dimension is because we are not aware of a closed-form expression beyond.

Following the pattern in section C.4, we want to show that the diagrammatic expansion equation (C15) order by order in the potential reproduces a known expression once this is written out order by order in potential. The difficulty here is similar to that in section C.4, namely that it is fairly easy to expand the known expression for the stationary density *without* the normalisation. Working in Fourier-space, we will once again write both the expansion and the normalisation in modes.

The first step is to characterise the expansion terms F and to bring them in a form that lends itself more naturally to a comparison to the field theory. This characterisation involves some rather involved manipulations. In a second step, we will then demonstrate that the resulting expansion agrees with the diagrammatic one.

The classical stationary solution of the Fokker-Planck equation (C3) of a drift-diffusion particle in one spatial dimension on a periodic domain and subject to a periodic potential defined so that $\Upsilon(x+L)=\Upsilon(x)$ for $x\in[0,L)$ is [53, 54],

$$\rho_0(x)=\mathcal{N}^{-1}Z_-(x)\int_x^{x+L}\mathrm{d}y\,Z_+(y)\quad\text{with}\quad Z_\pm(x)=\exp\left(\pm\frac{\Upsilon(x)-w_0x}{\mathsf{D}_t}\right), \tag{C51}$$

similar to equation (C27) defined with an explicit normalisation,

$$\mathcal{N}=\int_0^L\mathrm{d}x\,Z_-(x)\int_x^{x+L}\mathrm{d}y\,Z_+(y)\ . \tag{C52}$$

The density

$$\rho_0(x)=\mathcal{N}^{-1}\sum_{j=0}^{\infty}\frac{1}{L}\sum_{n=-\infty}^{\infty}\mathrm{e}^{\mathring{\imath}k_nx}F_j(k_n) \tag{C53}$$

can be written systematically in orders of the potential up to the normalisation to be determined below. If $F_j(k_n)$ is the term of order j in Υ, expanding $Z_\pm(x)=\mathrm{e}^{\mp w_0x/\mathsf{D}_t}\sum_n(\pm\Upsilon(x)/\mathsf{D}_t)^n/n!$ in equation (C51), immediately gives

$$F_j(k_n)=\sum_{i=0}^{j}\frac{(-1)^i}{i!}\frac{1}{(j-i)!}f_{j,i}(k_n)\quad\text{with}\quad f_{j,i}(k_n)=\int_0^L\mathrm{d}x\,\mathrm{e}^{-\mathring{\imath}k_nx}\left(\frac{\Upsilon(x)}{\mathsf{D}_t}\right)^i\mathrm{e}^{w_0x/\mathsf{D}_t}\int_x^{x+L}\mathrm{d}y\left(\frac{\Upsilon(y)}{\mathsf{D}_t}\right)^{j-i}\mathrm{e}^{-w_0y/\mathsf{D}_t}\ . \tag{C54}$$

An easy route to perform the Fourier transformation on the right is to split it into two and perform separate Fourier transformations of $(-\Upsilon(x)/\mathsf{D}_t)^i$ and of the second term, $\int_x^{x+L}\mathrm{d}y\ldots$ tying both together again by a convolution afterwards. While the first term produces essentially equation (C31), the second term involving the integral is more complicated. Writing however

$$\mathrm{e}^{-\mathring{\imath}k_nx+w_0x/\mathsf{D}_t}=\frac{1}{-\mathring{\imath}k_n+w_0/\mathsf{D}_t}\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{-\mathring{\imath}k_nx+w_0x/\mathsf{D}_t}\ , \tag{C55}$$

which is well-defined as $-\mathring{\imath}k_n+w_0/\mathsf{D}_t\neq0$ for all n by virtue of k_n and w_0 being real and $w_0\neq0$, allows the second integral to be removed by an integration by parts. Surface terms then drop out as $\Upsilon(x)$ is periodic. Following at first the pattern of equation (C41) the resulting Fourier series reads

$$\begin{aligned}f_{j,i}(k_n)=&\frac{1}{L}\sum_{n_0=-\infty}^{\infty}\left(\frac{1}{L\mathsf{D}_t}\right)^iL\sum_{n_1,\ldots,n_{i-1}}\Upsilon_{n_0-n_1}\ldots\Upsilon_{n_{i-2}-n_{i-1}}\Upsilon_{n_{i-1}}\\&\times\frac{1-\exp(-w_0L/\mathsf{D}_t)}{-\mathring{\imath}k_{n-n_0}+w_0/\mathsf{D}_t}\left(\frac{1}{L\mathsf{D}_t}\right)^{j-i}L\sum_{m_1,\ldots,m_{j-i-1}}\Upsilon_{n-n_0-m_1}\ldots\Upsilon_{m_{j-i-2}-n_{j-i-1}}\Upsilon_{n_{j-i-1}}\ .\end{aligned} \tag{C56}$$

This expression has some shortcomings that are mostly down to notation, which can be seen in the first sum by setting $i=0$ or in the second sum by setting $i=j$. In both cases, the sums are ill-defined, with the first sum running over indices $n_1,\ldots,n_{-1}$ for $i=0$ and similarly the last sum for $i=j$. Choosing $i=1$ or $i=j-1$ causes similar problems. However, equation (C54) allows for all of these choices. The problem is resolved by changing the indeces similar to equation (C42), first in the individual Fourier-transforms and then after tying them together in a convolution

$$f_{j,i}(k_n) = \frac{1}{(L\mathsf{D}_t)^j}\sum_{p_1,\dots,p_j}\Upsilon_{p_1}\dots\Upsilon_{p_j}L\delta_{p_1+\dots+p_j,n}\frac{1-\exp(-w_0L/\mathsf{D}_t)}{-\mathring{\imath}k_{p_1+\dots+p_{j-i}}+w_0/\mathsf{D}_t} \tag{C57}$$

with the convention of $k_{p_1+\dots+p_{j-i}} = 0$ for $i = j$, as can be verified by direct evaluation of the corresponding Fourier transform. Similarly, we demand $\delta_{p_1+\dots+p_j,n} = \delta_{0,n}$ for $j = 0$, so that $f_{0,0}(k_n) = L\delta_{0,n}(1-\exp(-w_0L/\mathsf{D}_t))\mathsf{D}_t/w_0$, confirmed by direct evaluation of equation (C54). We state in passing F_j for $j = 0,1$ by direct evaluation of equations (C54) and (C57),

$$F_0(k_n) = L\delta_{0,n}\frac{1-\exp(-w_0L/\mathsf{D}_t)}{w_0/\mathsf{D}_t} \tag{C58a}$$

$$F_1(k_n) = \frac{1}{\mathsf{D}_t}\Upsilon_n\left\{\frac{1-\exp(-w_0L/\mathsf{D}_t)}{-\mathring{\imath}k_n+w_0/\mathsf{D}_t} - \frac{1-\exp(-w_0L/\mathsf{D}_t)}{w_0/\mathsf{D}_t}\right\} \tag{C58b}$$

$$= \frac{\mathring{\imath}k_n\Upsilon_n}{w_0}\frac{1}{-\mathring{\imath}k_n+w_0/\mathsf{D}_t}\,. \tag{C58c}$$

We proceed by deriving a recurrence formula for F_j.

C.5.1. Properties of $F_j(k_n)$

Equation (C57) is to be used to compile $F_j(k_n)$ according to equation (C54),

$$F_j(k_n) = \sum_{i=0}^{j}\frac{(-1)^i}{i!}\frac{1}{(j-i)!}\frac{1}{(L\mathsf{D}_t)^j}\sum_{p_1,\dots,p_j}\Upsilon_{p_1}\dots\Upsilon_{p_j}L\delta_{p_1+\dots+p_j,n}\frac{1-\exp(-w_0L/\mathsf{D}_t)}{-\mathring{\imath}k_{p_1+\dots+p_{j-i}}+w_0/\mathsf{D}_t} \tag{C59}$$

which we rewrite for $j \geqslant 1$ as

$$F_j(k_n) = \sum_{i=1}^{j}\frac{(-1)^i}{i!}\frac{1}{(j-i)!}f_{j,i}(k_n) - \sum_{i=1}^{j}\binom{j}{i}\frac{(-1)^i}{j!}f_{j,0}(k_n) \tag{C60}$$

where the second term is the term for $i = 0$ which has been removed from the first sum and multiplied by a clever unity for $j \geqslant 1$,

$$1 = -\sum_{i=1}^{j}\binom{j}{i}(-1)^i \tag{C61}$$

as $(1-1)^j = 0$ for $j \geqslant 1$, so that

$$F_j(k_n) = \sum_{i=1}^{j}\frac{(-1)^i}{i!}\frac{1}{(j-i)!}\frac{1}{(L\mathsf{D}_t)^j}\sum_{p_1,\dots,p_j}\Upsilon_{p_1}\dots\Upsilon_{p_j}L\delta_{p_1+\dots+p_j,n}\left[\frac{1-\exp(-w_0L/\mathsf{D}_t)}{-\mathring{\imath}k_{p_1+\dots+p_{j-i}}+w_0/\mathsf{D}_t} - \frac{1-\exp(-w_0L/\mathsf{D}_t)}{-\mathring{\imath}k_{p_1+\dots+p_j}+w_0/\mathsf{D}_t}\right], \tag{C62}$$

using $\binom{j}{i}/j! = 1/(i!(j-i)!)$. The square bracket can be simplified further as $k_{p_1+\dots+p_j} = k_n$ by the Kronecker δ-function and

$$k_n - k_{p_1+\dots+p_{j-i}} = k_{p_{j-i+1}+\dots+p_j} = k_{p_{j-i+1}} + k_{p_{j-i+2}} + \dots + k_{p_j} \tag{C63}$$

so that

$$F_j(k_n) = \sum_{i=1}^{j}\frac{(-1)^i}{i!}\frac{1}{(j-i)!}\frac{1}{(L\mathsf{D}_t)^j}$$
$$\times\sum_{p_1,\dots,p_j}\Upsilon_{p_1}\dots\Upsilon_{p_j}L\delta_{p_1+\dots+p_j,n}\left[\frac{(1-\exp(-w_0L/\mathsf{D}_t))\left(-\mathring{\imath}\left(k_{p_{j-i+1}}+k_{p_{j-i+2}}+\dots+k_{p_j}\right)\right)}{\left(-\mathring{\imath}k_{p_1+\dots+p_{j-i}}+w_0/\mathsf{D}_t\right)\left(-\mathring{\imath}k_n+w_0/\mathsf{D}_t\right)}\right]. \tag{C64}$$

The last term in the numerator of the square bracket, $(-\mathring{\imath}(k_{p_{j-i+1}}+k_{p_{j-i+2}}+\dots+k_{p_j}))$, which is $(-\mathring{\imath})$ times equation (C63) can be split into i terms, resulting in i sums over $p_1,\dots,p_j$ for each i. But every sum is in fact equal, as the $p_1,\dots,p_j$ are dummy variables, so that the sum involving, say p_{j-i+1}, in the numerator can be turned into the sum involving p_j, simply by swapping the dummy variables p_{j-i+1} and p_j and then noticing that all other terms, such as $\Upsilon_{p_1}\ldots\Upsilon_{p_j}$ or $k_{p_1+\ldots+p_{j-i}}$ are invariant under such permutations. In fact, the indeces of the dummy variables divide naturally into two sets, namely $\{1,\ldots,j-i\}$ as used in $k_{p_1+\ldots+p_{j-i}}$ in one of the factors in the denominator, at the complement, $\{j-i+1,\ldots,j\}=\{1,\ldots,j\}\setminus\{1,\ldots,j-i\}$. In other words for $j\geqslant 1$

$$F_j(k_n)=\sum_{i=1}^{j}\frac{(-1)^i}{i!}\frac{1}{(j-i)!}\frac{1}{(L\mathsf{D}_t)^j}\sum_{p_1,\ldots,p_j}\Upsilon_{p_1}\ldots\Upsilon_{p_j}L\delta_{p_1+\ldots+p_j,n}\left[\frac{i\left(1-\exp(-w_0L/\mathsf{D}_t)\right)\left(-\mathring{\imath}k_{p_j}\right)}{\left(-\mathring{\imath}k_{p_1+\ldots+p_{j-i}}+w_0/\mathsf{D}_t\right)\left(-\mathring{\imath}k_n+w_0/\mathsf{D}_t\right)}\right] \tag{C65a}$$

$$=\frac{1}{L\mathsf{D}_t}\sum_{p_j}\frac{\mathring{\imath}k_{p_j}}{\left(-\mathring{\imath}k_n+w_0/\mathsf{D}_t\right)}\Upsilon_{p_j}\sum_{i=1}^{j}\frac{(-1)^{i-1}}{(i-1)!}\frac{1}{(j-i)!}\frac{1}{(L\mathsf{D}_t)^{j-1}} \tag{C65b}$$

$$\times\sum_{p_1,\ldots,p_{j-1}}\Upsilon_{p_1}\ldots\Upsilon_{p_{j-1}}L\delta_{p_1+\ldots+p_{j-1},n-p_j}\left[\frac{\left(1-\exp(-w_0L/\mathsf{D}_t)\right)}{\left(-\mathring{\imath}k_{p_1+\ldots+p_{j-i}}+w_0/\mathsf{D}_t\right)}\right]$$

$$=\frac{1}{L\mathsf{D}_t}\sum_{p_j}\frac{\mathring{\imath}k_{p_j}}{\left(-\mathring{\imath}k_n+w_0/\mathsf{D}_t\right)}\Upsilon_{p_j}\sum_{i=0}^{j-1}\frac{(-1)^{i}}{i!}\frac{1}{(j-1-i)!}\frac{1}{(L\mathsf{D}_t)^{j-1}} \tag{C65c}$$

$$\times\sum_{p_1,\ldots,p_{j-1}}\Upsilon_{p_1}\ldots\Upsilon_{p_{j-1}}L\delta_{p_1+\ldots+p_{j-1},n-p_j}\left[\frac{\left(1-\exp(-w_0L/\mathsf{D}_t)\right)}{\left(-\mathring{\imath}k_{p_1+\ldots+p_{j-1-i}}+w_0/\mathsf{D}_t\right)}\right]$$

$$=\frac{1}{L\mathsf{D}_t}\sum_{p_j}\frac{\mathring{\imath}k_{p_j}}{\left(-\mathring{\imath}k_n+w_0/\mathsf{D}_t\right)}\Upsilon_{p_j}F_{j-1}\left(k_n-k_{p_j}\right)\ , \tag{C65d}$$

where we have used the equivalence of the i terms in equation (C64) to write equation (C65a) which carries a factor of i in the numerator in the square bracket, taken the summation over p_j and other terms outside the rest of the expression in equation (C65b), shifted i by unity in equation (C65c), to finally re-express the sum as a convolution of a pre-factor with $F_{j-1}(k_n)$ using equation (C59). Equation (C65d) is the central result of thise section, providing a simple recurrence formula for $F_j(k_n)$ for all $j\geqslant 1$. We will use equation (C65d) in the following section to demonstrate the equivalence of the classical result equation (C53) and the field theoretic result equation (C15) with equation (C14) in the presence of drift in one dimension.

C.5.2. Relationship between $E_j(k_n)$ and $F_j(k_n)$

Similar to section C.4.2, we will now demonstrate that the density ρ_0 expanded in $F_j(k_n)$ according to equation (C53) with recurrence equation (C65d) and with normalisation equation (C52), is equal to that expanded in $E_j(k_n)$ according to equation (C15) and, in one dimension, (C22). We will do so by demonstrating that the jth order in Υ of $\mathcal{N}\rho_0$ with ρ_0 according to equation (C15) equals $F_j(k_n)$. Expressing $\mathcal{N}$ in terms of $F_j(k_n)$ from equations (C52) and (C53), this amounts to the task of showing

$$\sum_{i=0}^{j}F_i(0)\,E_{j-i}(k_n)=F_j(k_n)\ . \tag{C66}$$

similar to equation (C35), but now allowing for $w_0\neq 0$ and restricting ourselves to one dimension. Equation (C66) clearly holds for $j=0$, as

$$F_0(0)\,E_0(k_n)=L\frac{1-\exp(-w_0L/\mathsf{D}_t)}{w_0/\mathsf{D}_t}\delta_{n,0}=F_0(k_n) \tag{C67}$$

using equations (C16) and (C58a). It also holds for the more complicated $j=1$, equation (C58b),

$$F_1(0)\,E_0(k_n)+F_0(0)\,E_1(k_n)=\left(L\frac{1-\exp(-w_0L/\mathsf{D}_t)}{w_0/\mathsf{D}_t}\right)\left(-\frac{1}{L}\frac{k_n\Upsilon_n\mathcal{I}(n\neq 0)}{\mathsf{D}_tk_n+\mathring{\imath}w_0}\right)=\frac{\mathring{\imath}k_n\Upsilon_n}{w_0}\frac{1-\exp(-w_0L/\mathsf{D}_t)}{-\mathring{\imath}k_n+w_0/\mathsf{D}_t} \tag{C68}$$

using equations (C17) and (C58b) at $k_n=0$, the former in one dimension and the latter producing $F_1(0)=0$. In the last equality of equation (C68) we have dropped the indicator function as $k_n\mathcal{I}(n\neq 0)=k_n$, as the denominator has no zero at $k_n=0$ given that $w_0\neq 0$.

As in section C.4.2, we assume equation (C66) to hold for j and use equations (C22) and (C65d) to show in the following that equation (C66) holds for $j+1$. Writing therefore for $j \geqslant 0$

$$F_{j+1}(k_n) = (\mathcal{I}(n \neq 0) + \delta_{n,0}) F_{j+1}(k_n) \tag{C69a}$$

$$= \frac{\mathcal{I}(n \neq 0)}{L\mathrm{D}_t} \sum_q \frac{\mathring{\imath} k_{n-q}}{(-\mathring{\imath} k_n + w_0/\mathrm{D}_t)} \Upsilon_{n-q} F_j(k_q) + E_0(k_n) F_{j+1}(0) \tag{C69b}$$

as in equation (C48) using equation (C39) in the first line and in the second line using equation (C65d) with p_j replaced by $n-q$ to rewrite $F_{j+1}(k_n)$ and $\delta_{\mathbf{n},\mathbf{0}}$ replaced by $E_0(k_n)$ according to equation (C16). The $F_j(k_q)$ can now be replaced by equation (C66),

$$F_{j+1}(k_n) = \frac{\mathcal{I}(n \neq 0)}{L\mathrm{D}_t} \sum_q \frac{\mathring{\imath} k_{n-q}}{(-\mathring{\imath} k_n + w_0/\mathrm{D}_t)} \Upsilon_{n-q} \sum_{i=0}^{j} F_i(0) E_{j-i}(k_q) + E_0(k_n) F_{j+1}(0) \tag{C70}$$

and the convolution performed on $E_j(k_n)$, equation (C22), which gives

$$F_{j+1}(k_n) = \sum_{i=0}^{j} F_i(0) E_{j-i+1}(k_n) + E_0(k_n) F_{j+1}(0) = \sum_{i=0}^{j+1} F_i(0) E_{j+1-i}(k_n) \tag{C71}$$

confirming equation (C66) for $j+1$, provided it holds for j. With equation (C71) as the induction step and equation (C67) or (C68) as the base case, this confirms equation (C15) with (C22) in the case of drift diffusion in one dimension.

C.6. Summary

In the present appendix, we have introduced a general formula to determine the stationary density $\rho_0(\mathbf{x})$ equation (C15) digrammatically, recursively and perturbatively in the potential, equation (C21). We have validated this expression for the case of pure diffusion producing the barometric formula, equation (C27), in section C.4 and for the case of drift-diffusion in one dimension, equation (C51), in section C.5. In both cases, we have used induction to show the equivalence of the density derived from theory and the density derived from classical considerations. The key challenge is to compare the field theoretic terms to a certain order in the potential to the corresponding terms in the classical result, which is straight-forwardly expanded in powers of the potential only up to a normalisation, which needs to be expanded itself, equations (C34), (C35) and (C66).

In order to treat the potential perturbatively, we had to allow for vanishing potential, which allows for a stationary state only if the system is finite. However, the resulting perturbation theory reproducing the Boltzmann factor in the case of no drift means that it applies equally for *confining* potentials. This applies similarly to the case with drift, as the thermodynamic limit $L \to \infty$ may be taken after resumming the perturbative result into the integral expression equation (C51).

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