COMMUN. MATH. SCI.
Vol. 15, No. 2, pp. 539–554

ON EQUIPARTITION OF ENERGY AND INTEGRALS OF GENERALIZED LANGEVIN EQUATIONS WITH GENERALIZED ROUSE KERNEL*

CHRISTEL HOHENEGGER†

Abstract. We show that if the motion of a particle in a linear viscoelastic liquid is described by a Generalized Langevin Equation with generalized Rouse kernel, then the resulting velocity process satisfies equipartition of energy. In doing so, we present a closed formula for the improper integration along the positive line of the product of a rational polynomial function and of even powers of the sinc function. The only requirements on the rational function are sufficient decay at infinity, no purely real poles and only simple nonzero poles. In such, our results are applicable to a family of exponentially decaying kernels. The proof of the integral result follows from the residue theorem and equipartition of energy is a natural consequence thereof. Furthermore, we apply the integral result to obtain an explicit formulae for the covariance of the position process both in the general case and for the Rouse kernel. We also discuss a numerical algorithm based on residue calculus to evaluate the covariance for the Rouse kernel at arbitrary times.

Keywords. Residue calculus, generalized Langevin equations, equipartition of energy, covariance, improper integrals, Gaussian processes.

AMS subject classifications. 82C31, 30E20, 60G15, 60K40, 76A05.

1. Introduction

The one dimensional Langevin equation describes the motion of a neutrally buoyant particle of mass m and radius r in a viscous fluid of viscosity η_s under the influence of drag and thermal forces. With $\gamma_s = 6\pi\eta_s r$ the drag coefficient, it is known as an Ornstein-Uhlenbeck process and has the form

$$m\frac{\underset{\cdot}{V}(t)}{\underset{\cdot}{t}} = -\gamma_s V(s) + \sqrt{2k_B T\gamma_s}\,\dot{W}(t) \quad \mathbb{E}[\dot{W}(t)\dot{W}(s)] = \delta(t-s) \quad \frac{\underset{\cdot}{X}(t)}{\underset{\cdot}{t}} = V(t). \tag{1.1}$$

In Equation (1.1), k_B is the Boltzmann constant, T is the temperature and $\dot{W}$ is a time white noise. Since the exact solution for $V(t)$ is known (see [11, 12]), the stationary solution of the stochastic differential equation (1.1) satisfies

$$\mathbb{E}[V(0)^2] = \frac{k_B T}{m}. \tag{1.2}$$

In other words, the coefficient in front of $\dot{W}(t)$ in Equation (1.1) is such that equipartition of energy is satisfied. Furthermore, the covariance of both $V(t)$ and $X(t)$ can be explicitly calculated (using Itô's lemma). Both stochastic processes are Gaussian, but only $V(t)$ is Markovian. In this work, we consider similar questions for a fluid with memory on multiple time scales or viscoelasticity described by relaxation times.

A viscoelastic fluid is a liquid that exhibits both elastic and viscous properties, responding differently based on the applied stress. A neutrally buoyant spherical particle of mass m and radius r moving freely in such an environment is subject to viscous and elastic dissipation via drag forces and diffusion via thermal forces. In one dimension,

*Received: April 28, 2016; accepted (in revised form): October 12, 2016. Communicated by Chun Liu.
This work is partially supported by grant NSF DMS-1413378.
†Department of Mathematics, University of Utah, 155 S 1400 E Room 233, Salt Lake City, UT 84112-0090, USA(choheneg@math.utah.edu). http://www.math.utah.edu/ choheneg

the generalization of Newton's equation of motion to describe the displacement of the particle is achieved in the form of a Generalized Langevin Equation (GLE) for the particle velocity process $V(t)$ driven by a mean zero Gaussian process $F(t)$ (see [8, 13, 14, 15])

$$m\frac{V(t)}{t} = -\frac{\gamma_p}{\tau_{\text{avg}}}\int_{-\infty}^{\infty} K^+(t-s)V(s)ds + \sqrt{\frac{k_B T\gamma_p}{\tau_{\text{avg}}}}F(t) \quad \mathbb{E}[F(t)F(s)] = K(t-s). \tag{1.3}$$

Here $\gamma_p = 6\pi r\eta_p$ with η_p the polymeric fluid viscosity is the drag coefficient, τ_{avg} is the average relaxation time of the polymer and $K^+(t) = K(t)u(t)$ with $u(t)$ the unit step function accounting for causality in the integral is the memory kernel. We remark that analysis of the units dictates that the coefficient in front of the integral has units of mass per time squared and not mass per time. In this form, Equation (1.3) satisfies the fluctuation-dissipation theorem, that is the memory kernel $K(t)$ is linked to the fluctuations of the noise by the relationship $\mathbb{E}[F(t)F(s)] = K(t-s)$ [3]. In this paper, we only consider linear viscoelasticity and choose $K(t)$ to be the dimensionless Generalized Rouse kernel

$$K(t) = \frac{1}{N}\sum_{n=0}^{N-1} e^{-|t|/\tau_n} \qquad \tau_n = \tau_0\left(\frac{N}{N-n}\right)^2 n = 0,\ldots,N-1. \tag{1.4}$$

Equations (1.3) and (1.4) with $N = 1$ correspond to a viscoelastic fluid model whose stress is described by the upper Maxwell model, in other words where the solvent viscosity is zero. From Equation (1.3), the particle's position is calculated as the integral of the process,

$$X(t) = \int_0^t V(s)s \quad X(0) = X_0. \tag{1.5}$$

The goal of this paper is to show that in the above setting (1.3)-(1.5), $V(t)$ satisfies equipartition of energy and that closed formulae for the covariance of $X(t)$ can be found. This will be achieved via a general improper integral and careful integration in the complex plane. While we do not consider the effect of a harmonic force in this paper, our results can be seen as a generalization of the pioneering work of Kubo [4, 5] for a generalized Langevin equation for a particle under the influence of memory, a random and a harmonic force to a particle under the influence of a Gaussian force and memory on many scales. Finally, we remark that Kou [3] considered a similar set-up, but for a particle described by a GLE driven by fractional Brownian motion and showed that the resulting process satisfies equipartition of energy and is subdiffusive. The main difference between driving the GLE by fractional Brownian motion or by a Gaussian process $F(t)$ is that fractional Brownian motion is self-similar [7].

The paper is organized as follows. In Section 2, we set-up the questions in the form of certain improper integrals of a rational function $\Psi(x)$, which we derive. While we are motivated by the physical GLEs, the derivation applies to a generic GLE with exponentially decaying memory kernel. In Section 3, we present the main integral result for the improper integral $\int_0^\infty \Psi(x)\frac{\sin^a(x)}{x^a}x$ for a even. We assume that $\Psi(z)$ has sufficient decay at infinity in the complex plane and that the simple pole of $\Psi(z)$ are not real or zero. It is worth mentioning that if $\Psi(x) \equiv 1$, then the integrals in questions are simply sinc integrals for which closed and analytical formulae exist [10]. The proof uses techniques from residue calculus, contour integration and trigonometric power series expansion. We then show that $\Psi(x)$ constructed for a generic GLE with exponentially decaying memory kernel satisfies the assumptions of the main theorem. Next, we apply these results to derive explicit formulae for the stationary variance of $V(t)$ (Section 4) and for the covariance of $X(t)$ (Section 5). The proof of equipartition of energy in Section 4 is independent of N and of the choice of positive τ_n's. In Section 5, we present the numerical evaluation of the covariance for $N \leq 20$. Finally, Section 6 discusses similar integration formulae and extension to other physically motivated models.

2. General framework

In order to facilitate applications to other models, we consider the general GLEs

$$\frac{dY(t)}{dt} = -bK^{+} \star Y(t) + c\sqrt{b}F(t) \qquad \mathbb{E}[F(t)F(s)] = K(t-s) \tag{2.1}$$

$$\frac{dZ(t)}{dt} = Y(t), \tag{2.2}$$

where $Y(t)$ is not necessarily a velocity process and $b, c \in \mathbb{R}^{+}$. The physical GLEs (1.3) and (1.5) can be recovered with $Y = V$, $X = Z$, $b = \gamma_p/(\tau_{\text{avg}} m)$ and $c = \sqrt{k_B T/m}$. In the above, $\star$ denotes the time convolution and $K^{+}(t) = K(t)u(t)$ where $u(t)$ is the unit step function in accordance with the causality of the fluid's memory. For a sequence of positive relaxation times $\tau_0, \ldots, \tau_{N-1}$, we choose an equally weighted exponentially decaying kernel

$$K(t) = \frac{1}{N} \sum_{n=0}^{N-1} e^{-|t|/\tau_n}. \tag{2.3}$$

We make sense of a solution to Equation (2.1) in Fourier space. To do so, we take the non-unitary, angular frequency definition of the Fourier transform, denoted by $\hat{\cdot}$:

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} f(x) e^{-i\omega x} dx \qquad f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{f}(\omega) e^{i\omega x} d\omega.$$

We say that $Y(t)$ is a mild solution of Equation (2.1) if the Fourier transform of its covariance function $\rho_Y(t) = \mathbb{E}[Y(t)Y(0)]$ is

$$\widehat{\rho_Y}(\omega) = c^2 \frac{b\hat{K}(\omega)}{|i\omega + b\widehat{K^{+}}(\omega)|^2} = c^2 \Psi(\omega). \tag{2.4}$$

We remark that, formally, the auto-covariance of $Y(t)$ can be calculated because the exact solution of Equation (2.1) can be written as a convolution. For completeness, the calculation is presented next. Taking the Fourier transform of Equation (2.1) and solving for $\hat{Y}$, we have

$$\widehat{Y}(\omega) = \frac{\sqrt{c}b\widehat{F}(\omega)}{i\omega + b\widehat{K^{+}}(\omega)}. \tag{2.5}$$

Equation (2.5) implies that $Y(t)$ can be written as the convolution of F and a susceptibility kernel in the form

$$Y(t) = (\chi * F)(t) = \int_{-\infty}^{\infty} \chi(t-s) F(s) ds,$$

where $\widehat{\chi}(\omega) = \sqrt{c}b/(i\omega + b\widehat{K^{+}}(\omega))$. Plugging $Y(t)$ in the definition of the auto-covariance and using the definition of the covariance of $F(t)$ in Equation (2.1), we have

$$\rho_Y(t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \chi(t-s)\chi(-s')K(s-s')\underset{\cdot}{s}\underset{\cdot}{s}'.$$

Setting $u = s - s'$ in the above and integrating reveal the expression

$$\rho_Y(t) = \int_{-\infty}^{\infty} \left(\chi * \chi^{\dagger}\right)(t-u)K(u)\underset{\cdot}{u} = \left[\left(\chi * \chi^{\dagger}\right) * K\right](t)$$

where $\chi^{\dagger}(s) = \chi(-s)$ for all s. Since $\widehat{\chi^{\dagger}}(\omega) = \overline{\widehat{\chi}(\omega)}$, we find

$$\widehat{\rho}_Y(\omega) = |\widehat{\chi}(\xi)|^2 \widehat{K}(\omega) = c\frac{b^2\widehat{K}(\omega)}{|i\omega + b\widehat{K^{+}}(\omega)|^2}$$

in accordance with Equation (2.4).
Letting $\lambda_j = \tau_j^{-1}$, $j = 0, \cdots, N-1$, calculating $\hat{K}(\omega)$ and $\widehat{K^{+}}(\omega)$, and defining the fractional function $\Phi(x) = \frac{1}{N}\sum_{n=0}^{N-1} \frac{1}{x+\lambda_n}$, for $x \in \mathbb{R}$, we write Ψ as

$$\Psi(\omega) = \left[\frac{1}{\imath\omega + b\Phi(\imath\omega)} + \frac{1}{-\imath\omega + b\Phi(-\imath\omega)}\right]. \tag{2.6}$$

In the above, we used the fact that $\overline{\Phi(\imath\omega)} = \Phi(-\imath\omega)$, where $\bar{z}$ denotes the complex conjugate of z and that $\omega \in \mathbb{R}$.
With the convention $c^2 = k_BT/m$, showing that Equation (2.1) satisfies equipartition of energy is equivalent to showing that $\rho_Y(0) = \mathbb{E}[V(0)^2] = c^2$ or, using the Fourier transform and the fact that Ψ is even, that

$$\rho_Y(0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \widehat{\rho_Y}(\omega)\underset{\cdot}{\omega} = \frac{c^2}{\pi}\int_0^{\infty} \Psi(\omega)\underset{\cdot}{\omega} = c^2.$$

In other words, the equipartition of energy claims can be rewritten as

$$\mathcal{I}_1 := \int_0^{\infty} \Psi(\omega)\underset{\cdot}{\omega} = \pi. \tag{2.7}$$

Since $X(t)$ satisfies Equation (2.2), we know from the previous considerations that $X(t)$ is a Gaussian, non-stationary process with zero mean and covariance

$$\rho_Z(t,s) = \int_0^t \int_0^s \rho_Y(t'-s')\underset{\cdot}{s}'\underset{\cdot}{t}' \quad t > s.$$

Changing variables and reversing the order of integration, we have

$$\rho_Z(t,s) = tI_1(t) - (t-s)I_1(t-s) + sI_1(s) - [I_2(t) - I_2(t-s) + I_2(s)], \tag{2.8}$$

where $I_1(t) = \int_0^t \rho_Y(t')\underset{\cdot}{t}'$ and $I_2(t) = \int_0^t t'\rho_Y(t')\underset{\cdot}{t}'$ are the moments of $\rho_Y(t)$. Equation (2.8) can be further simplified when expressed using Fourier transforms. We find

$$\rho_Z(t,s) = J(t) + J(s) - J(t-s) \qquad J(t) = \frac{2}{\pi}\int_0^{\infty} \frac{\widehat{\rho_Y}(\omega)}{\omega^2}\sin^2\left(\frac{\omega t}{2}\right)\underset{\cdot}{\omega}. \tag{2.9}$$

With the definition of $\widehat{\rho_Y}(\omega)$ in Equation (2.4), evaluating $J(t)$ requires computing

$$\mathcal{I}_2(s) := \int_0^\infty \Psi(\omega)\frac{\sin^2(\omega s)}{\omega^2} \underset{\cdot}{\omega}. \tag{2.10}$$

Integrals $\mathcal{I}_1$ and $\mathcal{I}_2(s)$ are improper integrals of $\Psi(\omega)$ against power of the sinc function. Since $\Psi(0) = 2/(bN\tau_{\text{avg}})$, the integral is well-defined. In the next sections, we show that the integrals are finite. We start with a general integral result for $\int_0^\infty \Psi(\omega)\text{sinc}^a(\omega)\underset{\cdot}{\omega}$ for $a \geq 0$ even and $\text{sinc}(x) = \sin(x)/x$.

3. Integral result

As a convention, we denote by x a real variable, by z a complex variable, and we set $0^0 = 1$. Consider $\Psi(x)$, a rational polynomial function of the form $p(x)/q(x)$, such that $\deg(q) \geq \deg(p)+2$ and $q(x)$ has no purely real roots and only simple roots. The degree requirement is necessary to ensure proper decay of the function at infinity, while the location of the pole allows for a simple contour of integration. Further, let z_j for $j = 1,\ldots,M$ be the roots of $q(z)$ with positive imaginary parts, $\text{Im}(z_j) > 0$, $j = 1,\ldots,M$. Since $q(z)$ has no real roots, we have that $\deg(q) = 2M$. In order to prove the main theorem, we need a preliminary result from residue calculus.

Proposition 3.1. *Let $\Psi(x)$ be a rational polynomial function of the form $p(x)/q(x)$, such that $\deg(q) \geq \deg(p)+2$ and such that $q(x)$ has no purely real roots and only simple roots. Further, let $m, a \geq 0$ be integers and a be even. Then,*

$$\begin{aligned}
&\pi\imath \sum_{j=1}^{M}\left[\text{Res}(\Psi, z_j)\frac{e^{\imath m z_j}}{z_j^a} - \text{Res}(\Psi, \bar{z}_j)\frac{e^{-\imath m \bar{z}_j}}{\bar{z}_j^a}\right] - \pi\imath\Psi(0)\frac{(-\imath m)^{a-1}}{(a-1)!}\\
&= \int_{-R}^{-r}\frac{\Psi(x)}{x^a}\cos(mx)\underset{\cdot}{x} + \int_r^R \frac{\Psi(x)}{x^a}\cos(mx)\underset{\cdot}{x}\\
&\quad - \sum_{j=0}^{a/2-1}\frac{(-1)^j}{(2j)!}m^{2j}\int_{\Gamma_r}\frac{\Psi(z)}{z^{a-2j}}dz + O\left(r + \frac{1}{R^{a+1}}\right).
\end{aligned} \tag{3.1}$$

Here $\text{Res}(\Psi, z_j)$ denotes the residue of $\Psi(z)$ evaluated at z_j, $j = 1,\ldots,M$ and γ_r is the half-circle of radius r centered at the origin in the upper half-plane oriented clockwise. The radii r and R with $0 < r < R$ are chosen such that the region in the upper half plane bounded by above by the half-circle of radius R oriented clockwise and below by γ_r contains all the singularities of $\Psi(z)$ in the upper half-plane.

The proof is given in Appendix A. We note that more information about the form of $\Psi(\omega)$, as is the case for our intended applications, is needed to combine the residues. The next technical results about series can be found in tables of series, see for example [2, pages 134-137] or [1, section 0.15].

Lemma 3.1. *Let j,k be integers. If a is an even positive integer, then*

$$\sum_{j=0}^{a/2}(-1)^j\binom{a}{j}(a-2j)^{2k} = 0 \quad \textit{for all } k < \frac{a}{2}. \tag{3.2}$$

We can now state and proof the main integration theorem.

Theorem 3.1. *Let $\Psi(x)$ be an even rational polynomial function of the form $p(x)/q(x)$, such that $\deg(q) \geq \deg(p)+2$ and such that $q(x)$ has no purely real roots* *and only simple roots. Then, for $a \geq 0$ an even integer,*

$$\begin{aligned}\int_0^\infty \Psi(x)\operatorname{sinc}^a(x)\underset{\cdot}{x} = & \frac{\pi}{2^a}\sum_{k=0}^{a/2-1}(-1)^{k+1}\binom{a}{k}\Bigg[\frac{(-1)^{a/2}(a-2k)^{a-1}}{(a-1)!}\Psi(0) \\ & + \imath\sum_{j=1}^{M}\left(\operatorname{Res}(\Psi,z_j)\frac{e^{\imath(a-2k)z_j}}{z_j^a} - \operatorname{Res}(\Psi,\bar{z}_j)\frac{e^{-\imath(a-2k)\bar{z}_j}}{\bar{z}_j^a}\right)\Bigg] \\ & + \frac{\pi\imath}{2^{a+1}}\binom{a}{a/2}\sum_{j=1}^{M}\left(\operatorname{Res}(\Psi,z_j)\frac{1}{z_j^a} - \operatorname{Res}(\Psi,\bar{z}_j)\frac{1}{\bar{z}_j^a}\right).\end{aligned} \tag{3.3}$$

Fig. 3.1: *Region of integration. Let Γ_R be the circle of radius R and Γ_r the half-circle of radius r, both oriented counterclockwise and chosen to include all the poles of $\Psi(z)$.*

Proof. Consider the following contours of integration. Let $0 < r < R$, Γ_r be the half-circle connecting $-r$ to r in the upper half-plane oriented counterclockwise, and Γ_R be the circle of radius R oriented counterclockwise. Let $C^+ = [-R,-r] \cup (-\Gamma_r) \cup [r,R] \cup \Gamma_R^+$, where $+$ denotes the half-circle in the positive half-plane and the minus sign indicates reverse orientation. The radius r and R are chosen such that the region bounded by C^+ contains all the singularities of $\Psi(z)$ in the upper half-plane. Finally, let $C^- = \Gamma_R^- \cup (-[r,R]) \cup \Gamma_r \cup (-[-R,-r])$. The regions bounded by C^+ and C^- are sketched in Figure 3.1, where C^- is shaded in blue.

The proof relies on the trigonometric power expansion of $\sin^a(x)$ for a even,

$$\sin^a(x) = \frac{1}{2^a}\binom{a}{a/2} + \frac{1}{2^{a-1}}\sum_{k=0}^{a/2-1}(-1)^{k+1}\binom{a}{k}\cos((a-2k)x). \tag{3.4}$$

We first multiply Equation (3.4) by $\Psi(x)$, divide it by x^a and integrate it between r and R. Let $m = a-2k$. Since a is even and $\Psi(x)$ is even, we have

$$2\int_r^R \Psi(x)\frac{\cos(mx)}{x^a}\underset{\cdot}{x} = \int_{-R}^{-r}\Psi(x)\frac{\cos(mx)}{x^a}\underset{\cdot}{x} + \int_r^R \Psi(x)\frac{\cos(mx)}{x^a}\underset{\cdot}{x}.$$

Next, we apply Equation (3.1) to the resulting integrals to find

$$\begin{aligned}&\int_r^R \Psi(x)\operatorname{sinc}^a(x)\underset{\cdot}{x} \\ &= \frac{1}{2^a}\binom{a}{a/2}\int_r^R\frac{\Psi(x)}{x^a}\underset{\cdot}{x} + \frac{\pi}{2^a}\sum_{k=0}^{a/2-1}(-1)^{k+1}\binom{a}{k} \\ &\Bigg\{\imath\sum_{j=1}^{M}\left(\operatorname{Res}(\Psi,z_j)\frac{e^{\imath(a-2k)z_j}}{z_j^a} - \operatorname{Res}(\Psi,\bar{z}_j)\frac{e^{-\imath(a-2k)\bar{z}_j}}{\bar{z}_j^a}\right) - \frac{(a-2k)^{a-1}\Psi(0)}{(a-1)!} \\ &\quad + \frac{1}{\pi}\sum_{j=0}^{a/2-1}\frac{(-1)^j}{(2j)!}(a-2k)^{2j}\int_{\Gamma_r}\frac{\Psi(z)}{z^{a-2j}}\underset{\cdot}{z} + O\left(r + \frac{1}{R^{a+1}}\right)\Bigg\}.\end{aligned} \tag{3.5}$$

Applying Equation (3.1) with $m=0$ to the first integral on the right-hand side of Equation (3.5), substituting into Equation (3.5), grouping the sums involving residues and isolating the integral over Γ_r for $j=0$, we obtain

$$\begin{aligned}
&\int_r^R \Psi(x)\operatorname{sinc}^a(x)\underset{\cdot}{\mathrm{x}}\\
&=\frac{\pi 1}{2^{a+1}}\sum_{j=1}^{M}\Bigg\{\binom{a}{a/2}\left(\operatorname{Res}(\Psi,z_j)\frac{1}{z_j^a}-\operatorname{Res}(\Psi,\bar{z}_j)\frac{1}{\bar{z}_j^a}\right)\\
&\quad+2\sum_{k=0}^{a/2-1}(-1)^{k+1}\binom{a}{k}\left(\operatorname{Res}(\Psi,z_j)\frac{e^{\imath(a-2k)z_j}}{z_j^a}-\operatorname{Res}(\Psi,\bar{z}_j)\frac{e^{-\imath(a-2k)\bar{z}_j}}{\bar{z}_j^a}\right)\Bigg\}\\
&\quad+\frac{\pi}{2^a}\sum_{k=0}^{a/2-1}(-1)^k\binom{a}{k}\frac{(a-2k)^{b-1}}{(b-1)!}\Psi(0)\\
&\quad+\frac{1}{2^a}\Bigg\{\frac{11}{2}\left[-\binom{a}{a/2}+2\sum_{k=0}^{a/2-1}(-1)^k\binom{a}{k}\right]\int_{\Gamma_r}\frac{\Psi(z)}{z^a}\underset{\cdot}{\mathrm{z}}\\
&\quad+\sum_{k=0}^{a/2-1}(-1)^{k+1}\binom{a}{k}\sum_{j=1}^{a/2-1}\frac{(-1)^j}{(2j)!}(a-2k)^{2j}\int_{\Gamma_r}\frac{\Psi(z)}{z^{a-2j}}\underset{\cdot}{\mathrm{z}}\Bigg]+O\left(r+\frac{1}{R^{a+1}}\right)\Bigg\}.
\end{aligned}$$

Using $\binom{a}{k}=\binom{a}{a-k}$, the term in the square bracket in front of the integral over Γ_r of $\Psi(z)/z^a$ can be rewritten as

$$\begin{aligned}
&-\binom{a}{a/2}+2\sum_{k=0}^{a/2-1}(-1)^k\binom{a}{k}\\
&=(-1)^{a/2}\binom{a}{a/2}+\sum_{k=0}^{a/2-1}(-1)^k\binom{a}{k}+\sum_{k=0}^{a/2-1}(-1)^k\binom{a}{a-k}\\
&=(-1)^{a/2}\binom{a}{a/2}+\sum_{k=0}^{a/2-1}(-1)^k\binom{a}{k}+\sum_{j=a/2+1}^{a}(-1)^{a-j}\binom{a}{j}=\sum_{k=0}^{a}(-1)^k\binom{a}{k}=0.
\end{aligned}$$

In the above, we made use of the binomial identities $\sum_{k=0}^{a}(-1)^k\binom{a}{k}=0$ and of the fact that a is even. Finally, rearranging the terms in the sums involving the remaining integrals over Γ_r reveals a term of the form

$$\sum_{k=0}^{a/2-1}(-1)^k\binom{a}{k}(a-2k)^{2j}\quad j=1,\ldots,\frac{a}{2}-1.$$

By Lemma 3.1 this sum is zero. Letting $r\to 0$ and $R\to\infty$, the statement follows. ∎

We now verify that the hypothesis of Theorem 3.1 are satisfied for $\Psi(\omega)$ defined in Equation (2.6). From the construction of Ψ, we have $M=N+1$.

PROPOSITION 3.2. *Let $\Psi(\omega)$ be defined as in Equation* (2.6). *Then $\Psi(\omega)$ satisfies the assumptions of Theorem 3.1. In other words, $\Psi(\omega)$ is an even rational polynomial function of the form $p(x)/q(x)$ such that* $\deg(q)\geq\deg(p)+2$ *and $\Psi(\omega)$ has no purely real roots and only simple poles.*

Proof. From Equation (2.6), it is evident that $\Psi(\omega)$ is an even function. To show that $\Psi(\omega)$ satisfies the remaining properties, we express $\Psi(\omega)$ in terms of rational polynomials. To do so, let $\gamma = b/N$, and $p(x), q(x)$ be the polynomials

$$p(x) = \prod_{j=0}^{N-1}(x+\lambda_j) \quad q(x) = xp(x) + \gamma p'(x).$$

Here $'$ denotes the derivative of $p(x)$ with respect to x. Since $\deg(p) = N$, the degree of $q(x)$ is $N+1$. It is easy to see that $\Phi(\imath\omega) = p'(\imath\omega)/(Np(\imath\omega))$ and thus

$$\Psi(\omega) = \left[\frac{p(\imath\omega)}{q(\imath\omega)} + \frac{p(-\imath\omega)}{q(-\imath\omega)}\right]. \tag{3.6}$$

Furthermore, since the roots of $p(x)$ are $-\lambda_j < 0$, $j = 0, \ldots N-1$, the $N-1$ extrema of $p(x)$ are real and negative as well. Therefore, $q(x)$ has $N-1$ real negative roots located between extrema. Since $q(x)$ has an extrema between the largest root of $p(x)$ and zero, the last roots are either a pair of complex conjugate roots with non-zero imaginary part and negative real part if γ is not too small or two more purely negative roots if $\gamma \ll 1$. Therefore for γ not too small, the simple poles of $\Psi(\omega)$ in the upper half-plane are $N-1$ purely imaginary positive numbers ω_j, $j = 0, \ldots, N-2$, and a pair ω_{N-1}, ω_N of complex numbers with equal positive imaginary part and plus/minus real part. The other singularities are the complex conjugates in the lower half-plane. This guarantees that the denominator of $\Psi(\omega)$ has no purely real roots. A detailed discussion of the roots in the γ small and γ large limits is given in Appendix B.

It remains to show that the degree condition is satisfied. A-priori, the degree of the denominator in each fraction in Equation (3.6) is only one higher than the degree of the numerator. However, we show now that when the fractions are combined into a single fraction cancellation occurs. To combine the fractions, we replace $p(\imath\omega)$ and $q(\imath\omega)$ in Equation (3.6) by their series expansion obtained using Vieta's formula. We find

$$p(\imath\omega) = \imath^N \sum_{j=0}^{N}(-1)^j \omega^{N-j} t_j \quad q(\imath\omega) = \imath^{N+1} \sum_{j=0}^{N+1}(-1)^j \omega^{N+1-j} s_j,$$

where $s_j, j = 1, \ldots, N+1$ and $t_j, j = 1, \ldots, N$ are the elementary symmetric polynomials of the roots of $q(\imath\omega)$ (ω_j, $j = 0, \ldots, N$) and $p(\imath\omega)$ ($\imath\lambda_j$, $j = 0, \ldots, N-1$) respectively taken j at a time. Finally, plugging the above expressions into Equations (3.6) and (2.6) yields

$$\Psi(\omega) = \frac{1}{\imath}\left[\frac{\sum_{j=0}^{N}(-1)^j t_j \omega^{N-j}}{\sum_{j=0}^{N+1}(-1)^j s_j \omega^{N+1-j}} - \frac{\sum_{j=0}^{N} t_j \omega^{N-j}}{\sum_{j=0}^{N+1} s_j \omega^{N+1-j}}\right]. \tag{3.7}$$

Combining the fractions in Equation (3.7) reveals that the coefficient of the two highest monomials in the numerator are $t_0 s_0 - t_0 s_0 = 0$ and $2s_1 - 2t_1$, respectively. To conclude, we show that $s_1 = t_1$. This follows from the recurrence relationship between the coefficients:

$$t_0 = s_0 = 1 \quad t_1 = s_1 \quad t_j - \gamma(N-j+2)t_{j-2} = s_j \text{ for } 2 \le j \le N \quad -\gamma t_{N-1} = s_{N+1}, \tag{3.8}$$

which is obtained from substituting the series into $q(\imath\omega) = \imath\omega p(\imath\omega) + \gamma p'(\imath\omega)$. Thus the degree of the numerator is at most $2N-1$, while the degree of the denominator is $2N+2$, and the condition on the degrees of the polynomials is satisfied. $\square$

We will make use of the factorization in Equation (3.7) to compute residues of $\Psi(\omega)$.

4. Equipartition of energy

We now show that Equation (2.7) is true. Since $\Psi(\omega)$ satisfies the assumptions of Theorem 3.1 by Proposition 3.2, we apply it with $a=0$. Because $\Psi(\omega)$ has $N+1$ poles in the upper-half plane, application of Equation (3.3) with $a=0$ and $M=N+1$ yields

$$\int_0^\infty \Psi(\omega)d\omega = \frac{\pi 1}{2}\sum_{j=0}^{N}(\mathrm{Res}(\Psi,\omega_j)-\mathrm{Res}(\Psi,\bar{\omega}_j)). \tag{4.1}$$

With the factorization of $\Psi(\omega)$ derived in Equation (3.7), the residue's definition and the application of l'Hospital rule, the residues are

$$\mathrm{Res}(\Psi,\omega_j) = \frac{1}{1}\frac{\sum_{k=0}^{N}(-1)^k t_k \omega_j^{N-k}}{\sum_{k=0}^{N}(-1)^k s_k (N+1-k)\omega_j^{N-k}} \quad j=0,\dots,N. \tag{4.2}$$

Recalling from the proof of Lemma 3.2 that for γ not too small $\omega_j = iz_j$ with $z_j\in\mathbb{R}^+$ for $j=0,\dots,N-2$ and $z_{N-1,N}\in\mathbb{C}$ with $\mathrm{Re}(z_{N-1,N})>0$, we have that $\bar{\omega}_j=-\omega_j$ for $j=1,\dots,N-2$ and $\bar{\omega}_{N-1,N}=-\omega_{N,N-1}$. Therefore, using again the factorization (3.7) and the residue's definition, the rest of the residues are

$$\mathrm{Res}(\Psi,\bar{\omega}_j) = -\mathrm{Res}(\Psi,\omega_j)\ j=0,\dots,N-2 \quad \mathrm{Res}(\Psi,\bar{\omega}_{N-1,N}) = -\mathrm{Res}(\Psi,\omega_{N,N-1}).$$

We remark that for $\gamma\ll 1$, all the poles are purely imaginary and $\mathrm{Res}(\Psi,\bar{\omega}_j)=-\mathrm{Res}(\Psi,\omega_j)$, $j=0,\dots,N$. Finally, plugging into Equation (4.1), we have

$$\int_0^\infty \Psi(\omega)d\omega = \pi\sum_{j=0}^{N}\frac{\sum_{k=0}^{N}(-1)^k t_k\omega_j^{N-k}}{\sum_{k=0}^{N}(-1)^k s_k(N+1-k)\omega_j^{N-k}} = \pi\sum_{j=0}^{N} r_j, \tag{4.3}$$

where r_j, $j=0,\dots,N$ are the residues of the rational function $\tilde{p}(\omega)/\tilde{q}(\omega)$ with $\tilde{p}(\omega)=\sum_{k=0}^{N}(-1)^k t_k\omega^{N-k}$ and $\tilde{q}(\omega)=\sum_{k=0}^{N+1}(-1)^k s_k\omega^{N+1-k}$. This latest fact follows from the definition of the residues at ω_j, $j=0,\dots,N$, the simple roots of $\tilde{q}(\omega)$. Since $\deg(\tilde{p})=\deg(\tilde{q})-1$, the partial fraction decomposition of $\tilde{p}(\omega)/\tilde{q}(\omega)$ over $\mathbb{C}$ is

$$\frac{\tilde{p}(\omega)}{\tilde{q}(\omega)} = \frac{\displaystyle\sum_{k=0}^{N}(-1)^k t_k\omega^{N-k}}{\displaystyle\sum_{k=0}^{N+1}(-1)^k s_k\omega^{N+1-k}} = \sum_{j=0}^{N} r_j\frac{1}{\omega-\omega_j} = \frac{\displaystyle\sum_{j=0}^{N} r_j\prod_{\substack{k=0\\k\neq j}}^{N}(\omega-\omega_k)}{\displaystyle\prod_{j=0}^{N}(\omega-\omega_j)}.$$

In the right most expression, the coefficient of the highest degree monomial is $\sum_{j=0}^{N} r_j$, while the coefficient of the same monomial in $\tilde{p}(\omega)$ on the left is $t_0=1$. Therefore, we have $1=\sum_{j=0}^{N} r_j$, and combining this with Equation (4.3), we obtain

$$\mathcal{I}_1 = \int_0^\infty \Psi(\omega)\underset{\cdot}{\omega} = \pi,$$

as claimed in Equation (2.7). This result is independent of the positive τ_n's and of N,b,c.

REMARK 4.1. We remark that the above result about the variance of the stationary distribution, $\mathbb{E}[Y(0)^2]=c^2$, gives a natural rescaling the Gaussian process $Y(t)$ to another Gaussian process $\tilde{Y}$ that has unit variance. In other words, we seek $\tilde{Y}(t)$ and a modified GLE so that the stationary solution satisfies $\mathbb{E}[\tilde{Y}(0)^2]=1$. To do so, we define $t:=\tilde{t}/\sqrt{b}$, $c\tilde{Y}(\tilde{t}):=Y(t)$, $\tilde{K}(\tilde{t})=K(t)$ and we substitute it into the GLE (2.1). After dropping the tilde, Equations (2.1) and (2.3) become

$$\frac{\dot{\mathrm{Y}}(t)}{\dot{\mathrm{t}}}=-K^{+}\star Y(t)+F(t) \quad \mathbb{E}[F(t)F(s)]=K(t-s) \quad K(t)=\frac{1}{N}\sum_{n=0}^{N-1} e^{-\frac{|t|}{\sqrt{b}\tau_n}}.$$

This illustrates that under appropriate rescaling, Equation (2.1) can be written as a parameterless GLE.

5. Covariance

In order to apply Theorem 3.1 to $\mathcal{I}_2(s)$ in Equation (2.10), we change variable and let $y=s\omega$ to get

$$\mathcal{I}_2(s)=s\int_0^\infty \Psi\left(\frac{y}{s}\right)\mathrm{sinc}^2(y)\dot{\mathrm{y}}=s\int_0^\infty \Psi_s(y)\mathrm{sinc}^2(y)\dot{\mathrm{y}},$$

where $F_s(y)=F(y/s)$. Let y_j, $j=0,\dots,N$ denote the simple poles of $\Psi_s(y)$. From the definitions of $\Psi_s(y)$ and $\Psi(\omega)$, it follows that if y_j is a pole of $\Psi_s(y)$, then $\omega_j=y_j/s$ is a pole of $\Psi(\omega)$, $j=0,\dots,N$. Since $s>0$, the poles are in the upper-half plane and by construction and Proposition 3.2, $\Psi_s(y)$ satisfies the assumptions of Theorem 3.1. Thus, we calculate the residues of $\Psi_s(y)$ at y_j, $j=0,\dots,N$. We obtain

$$\mathrm{Res}(\Psi_s,y_j)=\lim_{y\to y_j}(y-y_j)\Psi_s(y)=s\mathrm{Res}(\Psi,\omega_j). \tag{5.1}$$

Since $\mathrm{Res}(\Psi,\overline{\omega_j})=\overline{\mathrm{Res}(\Psi,\omega_j)}$ for $j=0,\dots,N$ and all γ, and $\Psi_s(0)=\Psi(0)$, Equation 3.3 with $a=2$ yields

$$\mathcal{I}_2(s)=s\frac{\pi}{2}\left[\Psi(0)+\sum_{j=0}^{N}\mathrm{Im}\left(\frac{\mathrm{Res}(\Psi_s,y_j)}{y_j^2}\left(e^{2\imath y_j}-1\right)\right)\right].$$

Substituting Equation (5.1) into the previous expression, we find

$$\mathcal{I}_2(s)=\frac{\pi}{2}\left[s\Psi(0)+\sum_{j=0}^{N}\mathrm{Im}\left(\frac{\mathrm{Res}(\Psi,\omega_j)}{\omega_j^2}\left(e^{2\imath s\omega_j}-1\right)\right)\right], \tag{5.2}$$

where the residues are given by Equation (4.2). Unfortunately, no further simplifications of Equation (5.2) were found in the general case or in the γ small and large limits. We therefore discuss how this result can be used to numerically evaluate $\mathcal{I}_2(s)$ for our specific GLEs.

5.1. Application.

We consider again the GLEs (1.3) and (1.5) with a generalized Rouse kernel (1.4). Recall that in this case $c=\sqrt{k_BT/m}$ (units of length per time), $b=\gamma_p/(\tau_{\mathrm{avg}}m)$ (units of inverse time squared), and $\gamma_p=6\pi\eta_p a$. From the constitutive relationship of linear viscoelasticity [6] applied to the generalized Rouse kernel, we have $\eta_p=G_0\tau_{\mathrm{avg}}$, where G_0 is the mean stress. Plugging in yields $b=6\pi aG_0/m$, in other words b is independent of N, the number of kernels. We choose µm as unit of length, ms as unit of time, and mg as unit of mass. Polysterene bead tracers have a density of about $1.05\times10^{-9}\,\mathrm{mg\,\mu m^{-3}}$ close to that of water and a radius varying between $0.5\,\mu$m to $4\,\mu$m. For illustrative purpose, we choose $r=2\,\mu$m and calculate the mass as that of a sphere with the above density. Further, we set $G_0=1\times10^{-6}\,\mathrm{mg\,\mu m^{-1}\,ms^{-2}}$. This choice means that if $N=1$, then η_p is the same as the viscosity of water, while η_p for $N=20$ is about 32 times the viscosity of water. With these choices, γ ranges from $53.5\,\mathrm{ms}^{-2}$ to $1\times10^3\,\mathrm{ms}^{-2}$. Finally, we set $\tau_0=1\,$ms.

(a) $N=1$. (b) $N=30$.

Fig. 5.1: *Plot of the integrand $\Psi(\omega)\sin^2(\omega s)/\omega^2$ for the generalized Rouse kernel with $N=1$ (left) and $N=30$ (right) evaluated at $s=1\,$ms, $10\,$ms and $100\,$ms. As s increases the number of oscillations in the envelope (purple) $\Psi(\omega)/\omega^2$ increases.*

To compute the covariance of the position process $X(t)$, one as to evaluate $\mathcal{I}_2=\int_0^\infty \Psi(\omega)\sin^2(\omega s)/\omega^2 \d{s}$ as discussed in Section 2. Figure 5.1 shows the integrand, $\Psi(\omega)\sin^2(\omega s)/\omega^2$ as a function of ω for increasing values of s. The envelope is simply $\Psi(\omega)/\omega^2$. As s increases, the number of oscillations in the envelope increases drastically. We also note that the scale of y-axis in Figure 5.1 are different, which is to be expected from the construction of $\Psi(\omega)$.

The two factors affecting the numerical evaluation of $\mathcal{I}_2(s)$ using an adaptive scheme are the number of subintervals required as s increases and the cut-off of the integral at a large enough value to ensure accuracy. Table 5.1 shows a comparison between the computation time required for a numerical approximation of $\mathcal{I}_2(s)$ using an adaptive scheme and using Equation (5.2) to the same accuracy. The adaptive scheme is the built-in function INTEGRAL in Matlab R2015b. The new scheme uses Equation (5.2) to get a numerical approximation for $\mathcal{I}_2(s)$ provided that the poles $\omega_0,\dots,\omega_N$ can be found numerically. This last requirement naturally constrains how big $N+1$, the degree of the polynomial whose roots we are looking for, can be. However, for practical purposes, as N gets large the discrete relaxation spectrum can be replaced by a continuous spectrum and restricting ourselves to $N\le 20$ is reasonable. For sanity check, the information about the location of the roots for γ small and large gained in Appendix B is used to check the numerically computed roots and equipartition of energy (or the sum of the residues equals $-\imath$) is checked. The algorithm goes as follows.

(a) $s\in[0,10]$. (b) $s\in[0,100]$.

Fig. 5.2: *Plot of $\mathcal{I}_2(s)$ for the generalized Rouse kernel for short time $s\in[0,10]$ (left) and $s\in[0,100]$ (right) for $N=1$, 5, 10 and 20.*

(1) Let $\gamma=b/N$ and

$$\lambda_n=\frac{1}{\tau_0}\left(1-\frac{n}{N}\right)^2 \; n=0,\dots,N-1 \quad p(x)=\prod_{n=0}^{N-1}(x+\lambda_n) \quad q(x)=xp(x)+\gamma p'(x).$$

(2) Find $-z_1,\dots,-z_{M+1}$ the roots of $q(x)$. Let $\omega_j=\imath z_j$, $j=0,\dots,N+1$.

(3) Construct the symmetric polynomials $t_0,\dots,t_N$ for the polynomial with roots $i\lambda_n$, $n=0,\dots,N-1$ such that $p(\imath\omega)=\imath^N\sum_{j=0}^{N}(-1)^j\omega^{N-j}t_j$.

	Adaptive	Residue
$N=1$	13 s	0.05 s
$N=5$	23 s	0.01 s
$N=10$	24 s	0.006 s
$N=20$	25 s	0.005 s

Table 5.1: *Comparison of the computation times of $\mathcal{I}_2(s)$ at $s_j=j/100$, $j=0,\ldots,100$ between the Matlab R2015b built-in* INTEGRAL *adaptive scheme (left) and the residue algorithm described above (right) for $N=1$, 5, 10 and 20. The speed-up is due to the fact that the residues are only computed once independently of s.*

(4) Construct $s_0,\ldots,s_{N+1}$ such that $q(\imath\omega)=\imath^{N+1}\sum_{j=0}^{N+1}(-1)^j\omega^{N+1-j}s_j$ using the recurrence (3.8):

$$s_0=1 \quad s_1=t_1 \quad s_j=t_j-\gamma(N-j+2)t_{j-2} \text{ for } 2\le j\le N \quad s_{N+1}=-\gamma t_{N-1}.$$

(5) Evaluate the residues for $j=0,\ldots,N$ with Equation (4.2):

$$\operatorname{Res}(\Psi,\omega_j)=\frac{1}{\imath}\frac{\sum_{k=0}^{N}(-1)^k t_k\omega_j^{N-k}}{\sum_{k=0}^{N}(-1)^k s_k(N+1-k)\omega_j^{N-k}}.$$

(6) Evaluate the integral with Equation (5.2):

$$\mathcal{I}_2(s)=\frac{\pi}{2}\left[s\frac{2t_N}{\imath\gamma t_{N-1}}+\sum_{j=0}^{N}\operatorname{Im}\left(\frac{\operatorname{Res}(\Psi,\omega_j)}{\omega_j^2}\left(e^{2\imath s\omega_j}-1\right)\right)\right].$$

Most of the computation time of the above algorithm is spent in Steps 2 and 3, but these steps are independents of s and can therefore be precomputed. Evaluating Step 6 for each s is then fast. On the other hand, an adaptive scheme spends most of its computation time evaluating the integral for each desired s and since the integrand changes drastically as s each increases (see Figure 5.1), no information from a smaller s can be used in determining how many subintervals are needed. The expected speed-up of our algorithm over an adaptive scheme is summarized in Table 5.1. We note that the times were only computed for s up to 100 ms. In practice, one would want to find the covariance of $X(t)$, and thus generate paths, for a couple of seconds.

Finally, Figure 5.2 shows $\mathcal{I}_2(s)$ for $N=1$, 5, 10 and 20 for small s (left) and large s (right). We note that the y-axis are different between the two plots. For small s (left), the plot shows oscillations which is an effect of inertia in the system [9]. We also remark the strong difference between $N=1$ and $N=5$ and the smaller difference between $N=10$ and $N=20$. The latter is a further justification to limiting ourselves to maximum N of order 20-30.

6. Conclusion

We have derived a closed formulae for the improper integration along the positive line of the product of an even rational function $\Psi(\omega)$ of sufficient degree and without any real zeros and an even power of the sinc function using the residue theorem. The resulting expression is a sum over the residues of the a-priori known or numerically evaluated simple poles of $\Psi(\omega)$ and arises using the trigonometric power expansion of $\sin^a(x)$ for a even. It shows that $\int_0^\infty \Psi(\omega)\operatorname{sinc}^a(\omega)\dot{x}$ is finite and can be analytically calculated. A natural application of the integral result is used to show that the velocity process of a particle that is described by a Generalized Langevin Equation with an exponentially decaying kernel satisfies equipartition of energy, independently of the number of kernels, of the relaxation times, and of the coefficient in the GLE. A further application yielded an analytical expression for evaluating $\Psi(\omega)\sin^2(\omega s)/\omega^2$ along the positive real line as a function of s. When applied to the Rouse kernel, this latest result gave a numerical algorithm for a fast and accurate computation of the covariance of the position process without relying on an adaptive scheme. The integrals discussed in this paper cannot be computed using standard techniques like partial fraction decomposition or Fourier transforms. Finally, the numerical algorithm is limited by the computation of the roots of a (possibly) high degree polynomial, but the gain in computation time supersede such a limitation.

We have only considered a GLE where the solvent viscosity is zero and which is driven solely by a Gaussian process. However, our method, and in particular the proof of equipartition of energy, can be extended to a stochastic differential equation which includes both solvent and polymer viscosity and is driven by a Gaussian process $F(t)$ and a time white noise $\dot{W}(t)$. This model corresponds to a fluid satisfying the Oldroyd-B constitutive equation. Our results can also be naturally applied to a generalized Rouse kernel, where the exponent 2 in the definition of the τ_n's is replaced by α. An interesting question is then how to extend the proof of equipartition of energy to a kernel that does not have equally weighted coefficients $1/N$.

While we have only presented the integration result for a even, the residue method applies to a odd as well. The only differences being that the odd series expansion of $\sin^a(x)$ is required, as well as the analog of Proposition 3.1 with $\cos(mx)$ replaced by $\sin(mx)$ is needed. Furthermore, integrands of the form $\Psi(\omega)\sin^a(x)/x^b$ can also be treated with the residue calculus method described in this paper. In this case, the only adjustments are in the stopping point of the Taylor series of the exponential in the proof of Proposition 3.1 and the resulting adjustments in the statement of Theorem 3.1.

Appendix A. Proof of Proposition 3.1. Consider the contours of integration sketched in Figure 3.1. We show that Equation (3.1) holds by applying the residue theorem to the function $\Psi(z)\frac{e^{\imath mz}}{z^a}$ on C^+ and $\Psi(z)\frac{e^{-\imath mz}}{z^a}$ on C^-.

Since, the only singularities of the integrand $\Psi(z)\frac{e^{\imath mz}}{z^a}$ in C^+ are the pole of $\Psi(z)$, we apply the residue theorem to obtain

$$\oint_{C^+}\Psi(z)\frac{e^{\imath mz}}{z^a}\,dz = 2\pi\imath\sum_{j=1}^{M}\mathrm{Res}(\Psi,z_j)\frac{e^{\imath mz_j}}{z_j^a}. \tag{A.1}$$

Now, we consider each path integral on the semi-circles Γ_R^+ and Γ_r individually and bound them accordingly for $R\to\infty$ and $r\to 0$. Since $2M=\deg(q)\geq\deg(p)+2$, there exists some constant $C>0$ so that $|\Psi(z)|$ is bounded on Γ_R^+ by $C|z|^{-2}$. Therefore,

$$\left|\int_{\Gamma_R^+}\Psi(z)\frac{e^{\imath mz}}{z^a}\,dz\right|\leq\int_0^{\pi}\frac{C}{R^{a+1}}\,d\theta=\frac{C\pi}{R^{a+1}}=O\left(\frac{1}{R^{a+1}}\right)\quad a\geq 0. \tag{A.2}$$

On Γ_r, we expand $e^{\imath mz}$ as its Taylor series and write

$$e^{\imath mz}=\sum_{j=0}^{a-1}\frac{(\imath mz)^j}{j!}+(\imath mz)^a\sum_{j=0}^{\infty}\frac{(\imath mz)^j}{(j+m)!}.$$

After dividing by z^a, the leading order term in the above infinite sum is $O(1)$ so that the path integral over Γ_r is at least $O(r)$. Therefore, the integral over $-\Gamma_r$ becomes

$$-\int_{\Gamma_r} \Psi(z)\frac{e^{\imath mz}}{z^a}\mathrm{d}z = -\sum_{j=0}^{a-1}\frac{(\imath m)^j}{j!}\int_{\Gamma_r}\Psi(z)\frac{1}{z^{a-j}}\mathrm{d}z + O(r). \tag{A.3}$$

Next, breaking up the path integral over C^+ into its four piecewise components in Equation (A.1) and using Equations (A.2) and (A.3) we arrive at

$$\begin{aligned}2\pi\imath\sum_{j=1}^{M}\mathrm{Res}(\Psi,z_j)\frac{e^{\imath mz_j}}{z_j^a} &= \int_{-R}^{-r}\Psi(x)\frac{e^{\imath mx}}{x^a}\mathrm{d}x + \int_r^R \Psi(x)\frac{e^{\imath mx}}{x^a}\mathrm{d}x \\ &\quad -\sum_{j=0}^{a-1}\frac{(\imath m)^j}{j!}\int_{\Gamma_r}\Psi(z)\frac{1}{z^{a-j}}\mathrm{d}z + O\left(r+\frac{1}{R^{a+1}}\right).\end{aligned} \tag{A.4}$$

We now follow a similar procedure and apply the residue theorem to the function $\Psi(z)\frac{e^{-imz}}{z^a}$ and the contour C^-. The contour now contains the pole of order a of $1/z^a$ at $z=0$ and the singularities of $\Psi(z)$ with negative imaginary parts. Since $\Psi(z)$ is a rational polynomial functions, the poles of $\Psi(z)$ are simply $\bar{z}_j$, $j=1,\ldots,M$. Therefore, by the residue theorem, we have

$$\oint_{C^-}\Psi(z)\frac{e^{-\imath mz}}{z^a}\mathrm{d}z = 2\pi\imath\sum_{j=1}^{M}\mathrm{Res}(\Psi,\bar{z}_j)\frac{e^{-\imath m\bar{z}_j}}{\bar{z}_j^a} + 2\pi\imath\Psi(0)\mathrm{Res}\left(\frac{e^{-\imath mz}}{z^a},0\right). \tag{A.5}$$

Again, we estimate the path integrals over the semi-circles Γ_R^- and Γ_r. On Γ_R^-, the integral is $O\left(\frac{1}{R^{a+1}}\right)$ by the exact same argument as for the integral over Γ_R^+. On Γ_r, we proceed as before and expand e^{-imz} as its Taylor series. We find for the path integral

$$\int_{\Gamma_r}\Psi(z)\frac{e^{-\imath mz}}{z^a}\mathrm{d}z = \sum_{j=0}^{a-1}\frac{(-1)^j(\imath m)^j}{j!}\int_{\Gamma_r}\Psi(z)\frac{1}{z^{a-j}}\mathrm{d}z + O(r). \tag{A.6}$$

Therefore, breaking up the path integral over C^- into its four piecewise components in Equation (A.5), using Equation (A.6) and the bound on Γ_R^- yield

$$\begin{aligned}&2\pi\imath\sum_{j=1}^{M}\mathrm{Res}(\Psi,\bar{z}_j)\frac{e^{-\imath m\bar{z}_j}}{\bar{z}_j^a} + 2\pi\imath\Psi(0)\mathrm{Res}\left(\frac{e^{-\imath mz}}{z^a},0\right) \\ &= -\int_{-R}^{-r}\Psi(x)\frac{e^{-\imath mx}}{x^a}\mathrm{d}x - \int_r^R\Psi(x)\frac{e^{-\imath mx}}{x^a}\mathrm{d}x \\ &\quad +\sum_{j=0}^{a-1}\frac{(-1)^j(\imath m)^j}{j!}\int_{\Gamma_r}\Psi(z)\frac{1}{z^{a-j}}\mathrm{d}z + O\left(r+\frac{1}{R^{a+1}}\right).\end{aligned} \tag{A.7}$$

The last step is to calculate the residue of e^{-imz}/z^a at $z=0$. Because $z=0$ is a pole of order a of $1/z^a$, by definition, the residue is

$$\mathrm{Res}\left(\frac{e^{-\imath mz}}{z^a},0\right) = \frac{1}{(a-1)!}\frac{\mathrm{d}^{a-1}}{\mathrm{d}z^{a-1}}\left(e^{-\imath mz}\right)\Big|_{z=0} = -\frac{(\imath m)^{a-1}}{(a-1)!}. \tag{A.8}$$

Finally, plugging Equation (A.8) into Equation (A.7), we find

$$
\begin{aligned}
&2\pi\imath\left[\sum_{j=1}^{M}\operatorname{Res}(\Psi,\bar{z}_j)\frac{e^{-\imath m\bar{z}_j}}{\bar{z}_j^a}+\frac{(-\imath m)^{a-1}\Psi(0)}{(a-1)!}\right]\\
&=-\int_{-R}^{-r}\Psi(x)\frac{e^{-\imath mx}}{x^a}\underset{\cdot}{x}-\int_{r}^{R}\Psi(x)\frac{e^{-\imath mx}}{x^a}\underset{\cdot}{x}\\
&\quad+\sum_{j=0}^{a-1}\frac{(-1)^j(\imath m)^j}{j!}\int_{\Gamma_r}\Psi(z)\frac{1}{z^{a-j}}\underset{\cdot}{z}+O\left(r+\frac{1}{R^{a+1}}\right).
\end{aligned}
\tag{A.9}
$$

The equality (3.1) follows by subtraction Equation (A.9) from Equation (A.4) and combining the complex exponential into cosines.

Appendix B. Location of the roots. We discuss the location of the zeros of $q(\imath\omega)=\imath\omega p(\imath\omega)+\gamma p'(\imath\omega)$ in the cases when $\gamma\ll 1$ and $\gamma\gg 1$.
First, if $\gamma\ll 1$, we expand $\omega=\omega_0+\gamma\omega_1$, a zero of $q(\imath\omega)=\imath\omega p(\imath\omega)+\gamma p'(\imath\omega)$, to linear order in γ. Plugging in these definitions, using Taylor series, and comparing terms, we have for the $O(1)$ and $O(\gamma)$ terms

$$
\begin{aligned}
O(1):&\quad \omega_0=0 \quad\text{or}\quad \omega_0=\imath\lambda_n \quad n=0,\dots,N-1 \text{ and}\\
O(\gamma):&\quad \omega_1=\imath\frac{p'(\imath\omega_0)}{\imath\omega_0 p'(\imath\omega_0)+p(\imath\omega_0)}, \text{ respectively.}
\end{aligned}
$$

Therefore, for $\gamma\ll 1$ and up to order $O(\gamma^2)$, the roots of $q(\imath\omega)$ are all imaginary with positive imaginary parts. They are given by

$$
\omega_n=\imath\left[\lambda_n-\gamma\frac{1}{\lambda_n}\right]\; n=0,\dots,N-1 \quad \omega_N=\imath\left[\gamma\frac{p'(0)}{p(0)}\right].
$$

Second, if $\gamma=1/\varepsilon\gg 1$, we let $\omega=\omega_0+\varepsilon\omega_1$ and we note that $q(\imath\omega)$ can be rewritten as $q(\imath\omega)=\frac{1}{\varepsilon}[\varepsilon\imath\omega p(\imath\omega)+p'(\imath\omega)]$. Therefore, we seek a zero of $\varepsilon\imath\omega p(\imath\omega)+p'(\imath\omega)$. Using Taylor series and comparing terms, we find for the $O(1)$ and $O(\gamma)$ terms

$$
\begin{aligned}
O(1):&\quad \omega_0=\imath\kappa_n \quad p'(-\kappa_n)=0 \quad n=0,\dots,N-2, \text{ and}\\
O(\varepsilon):&\quad \omega_1=-\imath\kappa\frac{p(-\kappa_n)}{p''(-\kappa_n)} \quad n=0,\dots,N-2, \text{ respectively.}
\end{aligned}
$$

Since there are only $N-1$ zeroes of $p'(x)$ and the degree of $q(x)$ is $N+1$, we are missing a pair of complex conjugate roots. It can be found by letting $\omega=\omega_0+\varepsilon^\delta\omega_1$ with $\delta<0$ and looking for the highest possible power in ε. Plugging in and gathering term, we find that $\delta=-1/2$. Consequently, the two highest powers in $1/\varepsilon$ upon substitution in $\varepsilon q(\imath\omega)$ are $(N-1)/2$ and $(N-2)/2$. We find

$$
O(\varepsilon^{-(N-1)/2}):\omega_1=\pm\sqrt{N}, \text{ and } O(\varepsilon^{-(N-2)/2}):\omega_0=\frac{1}{2N}\sum_{n=1}^{N}\lambda_n.
$$

Thus, for $\gamma=1/\varepsilon\gg 1$ and up to order $O(\varepsilon)$, the roots of $\varepsilon q(\imath\omega)$ are

$$
\omega_n=\imath\kappa_n,\; p'(-\kappa_n)=0, n=0,\dots,N-2 \quad \omega_{N-1,N}=\frac{1}{2N}\sum_{n=1}^{N}\pm\sqrt{\frac{N}{\varepsilon}}.
\tag{B.1}
$$

REFERENCES

[1] I.S. Gradshteyn and I.M. Ryzhik, *Table of Integrals, Series and Products*, Academic Press, Seventh Edition, 2007.
[2] E. Hansen, *A Table of Series and Products*, Prentice Hall, 1975.
[3] S.C. Kou, *Stochastic modeling in nanoscale biophysics: Subdiffusion within proteins*, Ann. Appl. Stat., 2:501–535, 2008.
[4] R. Kubo, *The fluctuation-dissipation theorem*, Rep. Progr. Phys., 29:255–284, 1966.
[5] R. Kubo, *Statistical Physics II: Nonequilibrium Statistical Mechanics*, Springer, Second Edition, 1985.
[6] R.G. Larson, *Constitutive Equations for Polymer Melts and Solutions*, Butterworth–Heinemann, 1988.
[7] M. Lysy, N.S. Pillai, D.B. Hill, M.G. Forest, J.W.R. Mellnik, P.A. Vasquez, and S.A. McKinley, *Model comparison and assessment for single particle tracking in biological fluids*, J. Amer. Statist. Assoc., 111(516):1413–1426, 2016.
[8] T.G. Mason and D.A. Weitz, *Optical measurements of frequency-dependent linear viscoelastic moduli of complex fluids*, Phys. Rev. Lett., 74:1250–1253, 1995.
[9] S.A. McKinley, L. Yao, and M.G. Forest, *Transient anomalous diffusion of tracer particles in soft matter*, J. Rheology, 53:1487–1506, 2009.
[10] R.G. Medhurst and J.H. Roberts, *Evaluation of the integral* $I_n(b)=\frac{2}{\pi}\int_0^\infty\left(\frac{\sin x}{x}\right)^n\cos(bx)dx$, Math. Comp., 19:113–117, 1965.
[11] B. Øksendal, *Stochastic Differential Equations*, Springer, 2010.
[12] M. Scott, *Applied Stochastic in Science and Engineering*, Univerity of Waterloo, 2013.
[13] T.M. Squires and T.G. Mason, *Fluid mechanics of microrheology*, Annu. Rev. Fluid Mech., 42:413–438, 2010.
[14] K. Xu, M. Forest, and I. Klapper, *On the correspondence between creeping flows of viscous and viscoelastic fluids*, J. Nonnewton Fluid Mech., 145:150–172, 2007.
[15] R. Zwanzig, *Nonlinear generalized Langevin equations*, J. Stat. Phys., 9:215–220, 1973.