Functional Renormalisation Group for Brownian Motion II: Accelerated Dynamics in and out of Equilibrium

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Here we numerically solve the equations derived in part I of this two-part series and verify their validity. In particular we use the functional Renormalisation Group (fRG) flow equations to obtain effective potentials for initially highly anharmonic and non-polynomial potentials, including potentials with multiple trapping wells and barriers, and at different temperatures. The numerical computations determining the effective action are much faster than the direct simulation of the stochastic dynamics to which we compare our fRG results. We benchmark our numerical solutions to the flow equations by comparing the first two equilibrium cumulants from the fRG against the Boltzmann distribution. We obtain excellent agreement between the two methods demonstrating that numerical solutions for the effective potential can be accurately obtained in all the highly unharmonic cases we examined. We then assess the utility of the effective potential to describe the equilibrium 2-point correlation function $\langle x(0)x(t) \rangle$ and the relevant correlation time. We find that when Wavefunction Renormalisation is also utilized, these are obtained to percent accuracy for temperatures down to the typical height of the potentials’ barriers but accuracy is quickly lost for lower temperatures. We also show how the fRG can offer strong agreement with direct numerical simulation of the nonequilibrium evolution of average position and variance. Also, the fRG solution represents the whole ensemble average, further adding to its convenience over other techniques, such as direct numerical simulations or solving the Fokker-Planck diffusion equation, which require multiple solutions with different initial conditions to construct averages over an ensemble.

I. INTRODUCTION

In part one of this two part series we utilised one particular formulation of the Renormalisation Group [1], namely the functional Renormalisation Group (fRG) [2, 3]. We applied the fRG to Brownian Motion [4] and derived the flow equations [5] under two approximations of the fRG: the Local Potential Approximation (LPA) and Wavefunction Renormalisation (WFR). We showed how the solutions to these equations at $k = 0$ can have physical meaning, firstly to static quantities such as equilibrium position and variance, but also to dynamical properties. In particular we derived for the first time Effective Equations of Motion (EEOM) for the evolution of the average position, variance and covariance with full validity both in and out of equilibrium. This is a completely new approach in comparison to previous applications of the fRG to non-equilibrium physics [6–17]. In this second part we will present solutions to these equations from part one and verify their validity and predictive power for physical processes with the bonus that the fRG route for calculation is many orders of magnitude quicker than direct simulation of the random walk.

In Sec. [11] we present numerical solutions to the flow equations for five types of anharmonic bare potentials which represent highly non-trivial systems: a polynomial asymmetric potential which does not exhibit any local maxima, a symmetric quartic double well, an asymmetric, double Lennard-Jones with two local minima and a rather flat region around the maximum, as well as two "rugged" potentials consisting of a simple harmonic $x^2$ potential with the addition of gaussian bumps. We consider different temperatures, ranging from relatively high to comparable to the depth of the potential’s barriers, controlling the amplitude of fluctuations. Naturally, we find that the end results of the flow equations differ, with higher temperatures resulting in potentials that carry less memory of the bare potentials’ morphology. Using the obtained effective potentials $V_{k \to 0}$ we evaluate the mean position of the particle $\langle x \rangle$ and its variance $\langle x^2 \rangle - \langle x \rangle^2$ at equilibrium and find excellent agreement with the exact results from the equilibrium Boltzman distribution. This confirms that the numerical solution of the LPA flow equation is accurate for the the wide variety of potential shapes we have considered, at least around the minima of the effective potentials.

In Sec. [111] we verify that the equilibrium limit of the equations from part one are correct. In particular we verify that the LPA accurately predicts equilibrium position and variance correctly, which confirms the accuracy of our solution to the flow equations. We then examine the characteristic decay behaviour of the connected 2-
point function $\langle x(0) x(t) \rangle$ or covariance at equilibrium by utilizing both the effective potential $V_{k \rightarrow 0}$ and the WFR function $Z_{k \rightarrow 0}$, which is instead a test of the accuracy of the fRG formalism itself and in particular the LPA and WFR approximations. We evaluate how these fRG predictions compare to results from numerical simulations of the random walk and find very good agreement between them down to relatively low temperatures comparable to the height of the barriers in the potential. Where possible we also compare with the characteristic decay time obtained by exactly solving the corresponding Schrödinger equation (derived from the Fokker-Planck equation) for the lowest eigenvalue. We find that the the LPA + WFR fRG equations give a comparable match to the simulated decay rate at the percent level.

In Sec. IV we extend our results to non-equilibrium evolution. We present numerical solutions to the EEOM for the one- and two-point functions derived in part one. Our solutions to the EEOM are compared to both direct numerical simulation of equation (1) and the result from the evolution of the Fokker-Planck equation (31) where possible. We show the ability of the fRG to capture the non-trivial non-equilibrium evolution in these various potentials to reasonable accuracy outlining a new, competitive method to compute accelerated dynamics for this system of interest.

We conclude in Sec. V by summarising our main results and discuss possible future directions. In Appendix A we explicitly present the WFR solutions to the flow equation (5).

II. SOLUTIONS TO THE FLOW EQUATIONS

The physical system we are interested in is that of the overdamped Langevin equation:

$$\dot{x} = -\partial_x V(x) + \eta(t)$$

$$\langle \eta(t) \eta(t') \rangle = \Gamma \delta(t - t')$$

In this section we numerically integrate the flow equations for this system obtained in part one. These are for LPA:

$$\partial_k V_k(\chi) = \frac{\Gamma}{4} \cdot \frac{1}{k + \partial^2_\chi V_k(\chi)}$$

and for WFR:

$$\partial_k V_k(\chi) = \frac{\Gamma}{4} \cdot \frac{1}{k + \partial^2_\chi V_k(\chi)}$$

$$\partial_k \xi(\chi) = \frac{\Gamma}{4} \cdot \frac{\partial^2}{\xi(\chi) \cdot D^2}$$

We obtain the resulting effective potential and wave function renormalisation for five types of potentials:

1) A simple polynomial:

$$V(x) = x + \frac{x^2}{2} + \frac{\alpha x^3}{3} + \frac{x^4}{4}$$

with $g > 0$. ii) The doublewell:

$$V(x) = ax^2 + bx^4$$

with $a < 0$ and $b > 0$. iii) A doublewell made by two Lennard-Jones (LJ) potentials back to back:

$$V(x) = 4\epsilon_1 \left( \frac{\sigma^1_{12}}{(x + 3)^{12}} - \frac{\sigma^6}{(x + 3)^6} \right) + 4\epsilon_2 \left( \frac{\sigma^1_{12}}{(x - 3)^{12}} - \frac{\sigma^6}{(x - 3)^6} \right)$$

where $\sigma$ will be taken to be 1 from here on in and $\epsilon_1$ & $\epsilon_2$ represent the depth of each well. E.g. if $\epsilon_1 = \epsilon_2 = 1$ both wells are 1 unit deep (in $2D_0/\epsilon$ units) and the potential is symmetric. Clearly here the domain of interest is $x \in (-3, 3)$ as the potential diverges at $x = \pm 3$. We will also consider the scenario of a simple $x^2$ with additional gaussian bumps (or dips):

$$V(x) = x^2 + \sum_{i=1}^n \alpha_i \exp \left[ -\frac{(x - \beta_i)^2}{\mu} \right]$$

where there are $n$ bumps or dips with the prefactor $\alpha_i$ being positive or negative respectively. $\beta_i$ marks the location of each bump and $\mu$ the width of each bump which for simplicity we assume is the same for all. For our purposes we will focus on two variants of this setup: iv) An $x^2$ plus two bumps placed symmetrically away from the origin and v) an $x^2$ plus 3 bumps and 3 dips in an asymmetrical setup. This potential represents a rudimentary toy model for motion over a “potential energy landscape” with a series of local energy minima. The last two cases clearly demonstrate the effect of local extrema on the final shape of the effective potential since the underlying $x^2$ potential does not alter its shape under the RG flow.

The minima of the LPA effective potentials determine the equilibrium position of the particle in each case and their curvature at the minimum determines the variance. We find excellent agreement with the values obtained by the Boltzmann equilibrium distribution, allowing us to establish the accuracy of our numerical solution for the LPA flow equation. In the LPA approximation, the curvatures of the effective potentials around the minimum also determine the decay rates of the autocorrelation functions in equilibrium. We compare these with high accuracy numerical simulations of the stochastic process done using the open source software Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). We find that the LPA prediction alone leads to poorer agreement with simulations than the LPA + WFR prediction. In particular we find that, when wavefunction renormalisation is included, the autocorrelation decay rates for the potentials we study are quantitatively predicted by the fRG at the percent level above a certain temperature that we quantify.
Unless otherwise stated our chosen parameters will be:

\begin{align}
\text{Doublewell:} & \quad a = -1, \ b = 1/4 \\
\text{Poly:} & \quad g = 2 \\
\text{Unequal L-J:} & \quad \epsilon_1 = 1, \ \epsilon_2 = 10, \ \sigma = 1 \\
x^2 + 2 \text{ bumps:} & \quad \alpha_1 = \alpha_2 = 1.5, \ \mu = 0.06, \ \beta_1 = -\beta_2 = 1 \\
x^2 + 6 \text{ bumps/dips:} & \quad \alpha_1 = \alpha_4 = \alpha_5 = -1.5 \\
& \quad \alpha_2 = \alpha_3 = \alpha_6 = 1.5, \ \mu = 0.06 \\
& \quad \beta_1 = -\beta_2 = 0.7, \ \beta_3 = -\beta_4 = 1.4, \ \beta_5 = -\beta_6 = 2.1
\end{align}

expressed in units of $\varepsilon^2$ where we have chosen the reference temperature $2D_0 = 1/\varepsilon$ such that $x = \hat{x}$. This procedure essentially represents all physical quantities in terms of the fundamental timescale $\varepsilon$. Concretely this means the doublewell potential is (restoring the $\hat{\cdot}$ for clarity):

$$\hat{V}(\hat{x}) = -\varepsilon^2 \hat{x}^2 + \frac{1}{4} \varepsilon^2 \hat{x}^4 = \varepsilon^2 \left[ -\hat{x}^2 + \frac{1}{4} \hat{x}^4 \right]$$

As $\varepsilon$ is by necessity a small number we will plot these potentials in units of $\varepsilon^2$ later.

### 1. Polynomial Truncation

Before solving the full PDE \[3\] it is instructive to consider an approximation, focusing on the double well potential \[7\] for illustration. We consider a truncated polynomial ansatz for the effective potential $V_k(\chi)$ of the form

$$V_k(\chi) = E(k) + \sum_{i=1}^{N} \alpha_i(k)\chi^{2i}$$

with initial conditions defined such that it matches the original doublewell potential \[7\] at the cutoff:

$$E(k = \Lambda) = 0$$

(17)

$$\alpha_1(k = \Lambda) = a$$

(18)

$$\alpha_2(k = \Lambda) = b$$

(19)

and all coefficients of higher powers vanishing. We can then expand the r.h.s of \[3\] in powers of $\chi$, truncate the series at $2N$ and therefore write a set of $N + 1$ coupled ODEs in terms of the couplings that can then be solved numerically. Below we write the set of ODEs for the $O(4)$ truncation as it only concerns coupling coefficients up to order $x^4$:

$$\frac{dE(k)}{dk} = \frac{\Upsilon}{4} \left( \frac{1}{k + 2 \cdot \alpha_1(k)} - \frac{1}{k} \right)$$

(20)

$$\frac{d\alpha_1(k)}{dk} = -\frac{3\Upsilon \cdot \alpha_2(k)}{(k + 2 \cdot \alpha_1(k))^2}$$

(21)

$$\frac{d\alpha_2(k)}{dk} = \frac{36\Upsilon \cdot \alpha_4^2(k)}{(k + 2 \cdot \alpha_1(k))^3}$$

(22)

These equations show how the coefficients in the polynomial ansatz for the potential evolve when fluctuations of lower and lower frequencies are averaged over. Keeping more terms in the polynomial truncation is straightforward, leading to a hierarchy of flow equations for the different coefficients that can be easily obtained via a computer algebra software. Solving such polynomial flow equations is numerically much easier than solving the full PDE \[3\] and the solution to the full PDE should be approached as $N \to \infty$. However, this method is only well suited to initial potentials of polynomial form of small degree (e.g. the doublewell $-\hat{x}^2 + x^4/4$). For potentials with more complex shapes the full PDE must be solved.

The system of ODEs at each truncation was solved using Matlab’s built-in ode23s function which is based on a modified Rosenbrock formula of order 2. Focusing for concreteness on the variance and using equation \[27\], we can rewrite it as: \[27\] $\text{Var}(x) = \Upsilon/4\alpha_1(k = 0)$, showing naturally how the different coupling constants relate to physical quantities – the variance is inversely proportional to $\alpha_1(k = 0)$.

The results of this truncation for the doublewell potential are displayed in Fig. 1. Here we can see that the lowest order truncations match poorly with the correct value as given by the Boltzmann distribution. This discrepancy being particularly noticeable for $\Upsilon = 1$ with predictions of negative variance which is unphysical. However the value calculated by solving the full LPA PDE \[3\] is approached by including more terms with the $O(20)$ truncation matching the full PDE at both temperatures. The available thermal kinetic energy is $E_{th} = \Upsilon/2$ so $\Upsilon = 2$ corresponds to a thermal energy equal to the height of the doublewell barrier. We can therefore also think of $\Upsilon > 2$ corresponding to a high temperature regime, where the barrier can be overcome, and $\Upsilon < 2$ to a low temperature regime where trapping in one of the two minima occurs.

We see that, in this example at least, the polynomial approximation to the flow equations offers a viable option.

![Fig. 1: The convergence of the truncated system of ODEs to the full LPA PDE value for $\text{Var}(x)$ at equilibrium for $\Upsilon = 10$ (red) and $\Upsilon = 1$ (blue). $\text{Var}(x)$ as calculated from the Boltzmann distribution is also included for reference.](image)
FIG. 2: The flow of the polynomial Langevin potential $V$ in the LPA for $\Upsilon = 10$ (High temperature/strong fluctuations - top) and $\Upsilon = 1$ (Low temperature/Weak fluctuations - bottom). The blue curve indicates the bare potential which is progressively changed, through green and yellow, into the red effective potential, as fluctuations are integrated out.

to solving the flow, with the added bonus that it can be solved much quicker than the full LPA PDE. However, if the initial potential is not well approximated by a polynomial such as the Unequal-Lennard Jones, or our bumpy potentials, then one is forced to solve the full LPA PDE. Furthermore, computing the autocorrelation decay rate requires one to go beyond the LPA and include WFR, doubling the complexity of any polynomial truncation. We therefore now turn to the full PDEs, the numerical solution to which is both feasible and accurate as we demonstrate.

2. Full PDEs

We solve the LPA flow equation on a grid in the $\chi$ direction, using Matlab’s built in ode45 or ode15s function to evolve in the $k$ direction, depending on the potential. For most potentials ode45 – which is based on an adaptive step size Runge-Kutta method – was sufficient.

A similar approach was used for including (5). The numerical derivatives in the $\chi$ direction were based on a finite difference scheme using the Fornberg method with a stencil size of 5 for the potentials under study. While increasing the grid size improves the accuracy of the numerical derivative it also increases the number of coupled ODEs to be solved, making the integration much more computationally expensive. A balance must be drawn depending on the potential in question. We considered 1001 points with $x \in (-3, 3)$ for the ULJ and $x \in (-5, 5)$ for the rest. As mentioned above Figs. 2-6 are displayed in units where $x = \hat{x}$ ($2D_b = 1/\varepsilon$) and the vertical axis is expressed in units of $\varepsilon^2$. We have also expressed $k$ in units of $\varepsilon$. This is done such that the plotted flow of the dimensionless potential $\hat{V}_k(\hat{x})$ looks the same as of the dimensionful potential $V_k(x)$. Therefore even though this section will use $V(x)$ and $k$ to refer to the dimensionless parameters in units of $\varepsilon^2$ and $\varepsilon$ respectively they could just as easily be the dimensionful versions which we explicitly obtain by setting $\varepsilon \rightarrow 1$.

Our first example of a flow from the bare to the effec-
The flow of the unequal L-J Langevin potential $V$ in the LPA for $\Upsilon = 10$ (top) and $\Upsilon = 1$ (bottom). Again, the bare potential is denoted by the blue curve and the $k = 0$ effective potential by the red one.

The flow in the range $k \in (0.01, 600)$ is rather inconsequential and there is not much change in the shape of the potential. As $k \to 0$ is approached however, a distinct single minimum develops indicating the average position of the particle. As expected, the lower the temperature, the closest the effective minimum is to the bare potential’s minimum, indicating the relative weakness of fluctuations to force the particle to spend time away from it.

A perhaps more interesting case is shown in Fig. 3, displaying how the double well potential flows with renormalisation scale $k$ to its effective incarnation for high $\Upsilon = 10$ and low $\Upsilon = 1$ temperature. Again, for the high temperature in the range $k \in (0.01, 600)$ there is not much change in the shape of the potential. Physically this means that the fluctuations we have integrated out in this range do not contribute significantly to the particle moving between the two minima, only displacing the particle about each of the two distinct minima. However, by $k = 0.001$ the energy barrier has gotten significantly smaller meaning that we have started to integrate over fluctuations that drive the particle over the barrier. Naturally, when $k = 0$ is reached the potential is fully convex (as it must be by definition of $\Gamma$) with no barriers to overcome. Similar behaviour is obtained where again we consider the lower temperature, $\Upsilon = 1$. As one might expect it takes ‘longer’ in $k$ evolution for the barrier to disappear as fluctuations at each $k$ scale have less energy than their equivalent for the $\Upsilon = 10$ case. Of note is that not only is the evolution different but the final shape of $V_{k=0}(x)$ is different for the two different temperature regimes. For $\Upsilon = 1$ it is clear that the potential is much flatter around the origin than for $\Upsilon = 10$. This is suggestive of longer time scales required at lower temperatures to overcome the energy barrier and reach equilibrium. It also indicates longer times for the connected 2-point function to decay, as we discuss below.

Also of note is that for both cases the global minimum shifts from its degenerate values at $\pm \sqrt{2}$ to $x = 0$. This makes physical sense as one expects that the particle will spend most of its time at the bottom of each well so that its average position will be in the middle i.e. at the

FIG. 5: The flow of the $x^2$ potential with two additional bumps for $\Upsilon = 10$ (top) and $\Upsilon = 1$ (bottom). As before, the bare potential is denoted by the blue curve and the $k = 0$ effective potential by the red one.
FIG. 6: The flow of the $x^2$ potential with 3 additional gaussian bumps and 3 dips in the LPA for $\Upsilon = 10$ (top) and $\Upsilon = 1$ (bottom). As before, the bare potential is denoted by the blue curve and the $k = 0$ effective potential by the red one.

FIG. 4: The flow of the $x^2$ potential with with 3 additional gaussian bumps and 3 dips in the LPA for $\Upsilon = 10$ (top) and $\Upsilon = 1$ (bottom). As before, the bare potential is denoted by the blue curve and the $k = 0$ effective potential by the red one.

III. EQUILIBRIUM RESULTS

Using the equations of static equilibrium quantities derived in part one we can verify the validity of our numerical routines employed in the previous section by comparing to the predictions from the Boltzmann distribution. After we have verified this we can compare our prediction for the evolution of the covariance in equilibrium given by (28) to direct numerical solutions of the Langevin equation (1).

A. Equilibrium position

As we discussed in part one the minimum of the effective potential at $k = 0$ corresponds to the average position of the particle in equilibrium:

$$\partial_\chi V_{k=0}(\chi_{eq}) = 0$$  \hspace{1cm} (23)

Here we verify that this is indeed the case by comparing the position of these minima to that computed directly from the Boltzmann distribution. The agreement provides a check of the accuracy of the numerical solution to (3).
FIG. 7: The value of $\chi_{eq}$ for different values of the thermal energy $\Upsilon$ in the polynomial potential as calculated via the LPA. The original bare polynomial Langevin potential is plotted (not to scale) in blue for context.

| Potentials      | $\Upsilon$ | Boltz | LPA   |
|-----------------|------------|-------|-------|
| Polynomial      | 10         | -0.9618 | -0.96 |
|                 | 2          | -1.3227 | -1.33 |
|                 | 1          | -1.5170 | -1.52 |
| Unequal L-J     | 10         | 0.4854  | 0.485 |
|                 | 2          | 1.8522  | 1.85  |
|                 | 1          | 1.8684  | 1.87  |
| $x^2$ plus 6 bumps/dips | 5 | 0.0531  | 0.055 |
|                 | 2          | 0.1597  | 0.16  |

**TABLE I:** $\chi_{eq}$ as calculated from the Boltzmann distribution and the LPA effective potential.

Let us consider the (normalised) equilibrium Boltzmann distribution defined in the standard way:

$$P(x) = N \exp \left( -\frac{2V(x)}{\Upsilon} \right)$$ \hspace{1cm} (24)

where $N$ is chosen so that $\int_{-\infty}^{\infty} P(x) = 1$. We can then compute $\chi_{eq}$ in the standard way from the equilibrium probability distribution function:

$$\int_{-\infty}^{\infty} x \cdot P(x) = \chi_{eq}$$ \hspace{1cm} (25)

Looking at Table. I we can see that the LPA matches the Boltzmann distribution extremely well for a wide range of different potentials across the range of temperatures we examined. In Figs. 7 & 8 we have plotted the LPA prediction for the average position as the thermal energy $\Upsilon$ of the system is lowered and the equilibrium position shifts closer to the original potential’s minimum. This is particularly stark in Fig. 8 as it is clear at high temperature the equilibrium position is in the middle of the two wells suggesting a roughly symmetric Boltzmann distribution. However as temperature is lowered the $\chi_{eq}$ moves into the deeper well indicating that particles at equilibrium at low temperatures would nearly always be in this region as one would expect. Table II verifies that the numerical solution to the LPA flow equation (3) is accurate in capturing this crucial physical aspect of the system at equilibrium.

### B. Variance

| Potentials      | $\Upsilon$ | Boltz | LPA   |
|-----------------|------------|-------|-------|
| Polynomial      | 10         | 1.5690 | 1.569 |
|                 | 2          | 0.5931 | 0.5894|
|                 | 1          | 0.2938 | 0.2922|
| Doublewell      | 10         | 2.2198 | 2.2199|
|                 | 2          | 1.6655 | 1.6655|
|                 | 1          | 1.7043 | 1.7042|
| Unequal L-J     | 10         | 1.6858 | 1.6860|
|                 | 2          | 0.01426| 0.01962|
|                 | 1          | 1.0809 \cdot 10^{-3} | 1.02726 \cdot 10^{-3} |
| $x^2$ plus 2 bumps | 10 | 2.5317 | 2.5759|
|                 | 2          | 0.4145 | 0.4145|
|                 | 1          | 0.1554 | 0.1554|
| $x^2$ plus 6 bumps/dips | 5 | 1.2550 | 1.2551|
|                 | 3          | 0.7824 | 0.7813|
|                 | 2          | 0.5497 | 0.5499|

**TABLE II:** $\text{Var}(x)$ as calculated from the Boltzmann distribution and the LPA effective potential.

The fRG also allows for the computation of the variance of the equilibrium distribution, defined by:

$$\int_{-\infty}^{\infty} (x - \chi_{eq})^2 \cdot P(x) = \text{Var}(x)$$ \hspace{1cm} (26)
with the fRG predicting it to be

\[ \text{Var}_{eq}(x) = \frac{\Upsilon}{2V_{\chi\chi}} \]  

(27)

Clearly, the variance is related to how flat the \( k = 0 \) potential is near the minimum, controlled by \( V_{\chi\chi} \) at the equilibrium point. Unsurprisingly, the bigger the curvature of the effective potential, the smaller the variance for a fixed temperature. If variance changed linearly with temperature we can see from (27) that \( V_{\chi\chi} \) would not change as temperature was varied. However this variance does not generically scale linearly with temperature which is why the \( k = 0 \) curves in Figs. 2, 3 & 6 are generically flatter about the equilibrium point for \( \Upsilon = 1 \) than for \( \Upsilon = 10 \) in order to accommodate the fact that the equilibrium variance decreases by less than a factor of 10 for \( \Upsilon = 10 \rightarrow 1; V_{\chi\chi} \) near the equilibrium point must decrease as temperature is lowered. However in Figs. 4 & 5 the \( \Upsilon = 10 \rightarrow 1 \) transition marks a bigger transition in equilibrium behaviour due to the particle at equilibrium being now mostly trapped in one well instead of spread out over multiple. This means that the variance decreases by more than a factor of 10 as \( \Upsilon = 10 \rightarrow 1 \) and therefore \( V_{\chi\chi} \) near the equilibrium point must increase as temperature is lowered resulting in a steeper curve at \( k = 0 \). The takeaway point is that lowering temperature in a particular range can generically make the effective potential flatter or steeper around the minimum depending on the scaling of variance with temperature in that regime.

Either way, once the fRG flow equations have been solved, calculating the curvature of the effective potential at the minimum is very straightforward. Our results are summarised in Table. III and it is clear that the LPA offers very good agreement for the variance of the equilibrium distribution for all the potentials examined. This is as it should, see Appendix B or part one, and, conversely, offers a check that the numerical solution to the LPA equation is accurate. In the following subsection we will see what else the effective potential can tell us about the system that is not immediately available from the Boltzmann distribution.

C. Covariance

In addition to the static variance at equilibrium, the curvature of the effective potential around the minimum also determines the time dependence of correlations in equilibrium, quantified by the time dependent covariance or connected 2-point function

\[ \text{Cov}_{eq}(x(t_1)x(t_2)) = \frac{\Upsilon}{2V_{\chi\chi}} e^{-\lambda|t_1-t_2|} \]  

(28)

where \( \lambda \) is given in part one and for the LPA corresponds to \( V_{\chi\chi} \). Furthermore, now the solution to the WFR flow equation (5) for \( \zeta_{\chi} \) also contributes, providing a correction to the decay rate \( \lambda \). The full numerical solutions to (5) for the potentials considered here are described in detail in Appendix A.

In Table. III we collect the values of \( \lambda \) obtained using the fRG under LPA & WFR for different \( \Upsilon \) values, higher or comparable to the typical depth or barrier heights of the different potentials, and compare this directly to high accuracy numerical simulations of the Langevin equation (1) using LAMMPS. Where possible we also computed the first non-zero eigenvalue \( E_1 \) by diagonalising the Hamiltonian from the Schrödinger (or rescaled Fokker-Planck) equation in (31). We can clearly see from Table. III that for our potentials the value obtained via the LPA tends to deviate by \( \sim 10\%-15\% \) from the simulation value. Inclusion of the WFR factor \( \zeta_{\chi} \) reduces the deviation substantially error to \( \sim 1\%-5\% \) from the value obtained in the simulations. We plot the decay of the covariance at equilibrium for our five potentials of interest in Figs. 9, 10, 11, 12 & 13 as calculated by fRG techniques compared to direct numerical simulations of the langevin equation. For a polynomial potential, as
shown in Fig. 9 we can see how the decay rate as calculated via the fRG for both LPA and LPA + WFR closely matches the simulations at both high and low temperature. Fig. 10 shows the decay in the doublewell which at \( \Upsilon = 10 \) (top plot) shows great agreement with the simulation and Schrödinger calculation of \( \lambda \) with fRG methods. At \( \Upsilon = 2 \) (bottom plot) of Fig. 10 however we can see that the LPA is poorly capturing the correct decay rate and the improvement gained by including WFR offers is much more dramatic. The calculation of \( E_1 \) from the Schrödinger equation has proved a non-trivial numerical exercise for our unequal Lennard-Jones potential hence its omission from Table. III and Fig. 11. Here the fRG offers a very real advantage over more conventional methods to calculating this decay rate as we do not have to develop special numerical routines for every potential of interest, we simply solve the same two flow equations (3) \& (5). We can see in Fig. 11 how the LPA + WFR decay rate closely matches the simulated decay at high temperature with the advantage of being calculated much more quickly than the direct simulation. Even just the LPA decay at low temperature as seen in Table. III puts us in the correct ballpark for the decay rate.

For our \( x^2 \)-plus-bumps potentials the decay rate is shown for two and 6 bumps/dips in Figs. 12 \& 13 respectively and as in the ULJ case the computation of eigenvalues for these potentials is a non-trivial exercise. We can see in the top plot (\( \Upsilon = 10 \)) of Fig. 12 that the LPA and WFR both in good agreement with simulations and in the bottom plot (\( \Upsilon = 1 \)) the two decays correctly
vastly different from the bare highly non-trivial systems where the simulated decay is WFR decay at late times. This indicates that even for simulated decay with the simulations asymptoting to the LPA and WFR predictions appropriately bound the small that higher order eigenvalues would dominate the decay at earlier times. We speculate that this is the reason for the simulated decay not following a true exponential in all cases and emphasizes the inadequacy of $E_1$ to accurately describe covariance for all systems of interest. As LPA matches the decay rate predicted by the Boltzmann distribution and WFR is closer to the decay predicted by $E_1$ it is apparent why having both is highly useful and why it is nice to be able to get both in the same framework.

### IV. ACCELERATED DYNAMICS OUT OF EQUILIBRIUM

In order to solve the equations of motion for the one point function $\chi(t)$ and two point function $G(t,t')$ we must first solve the PDEs for the LPA & WFR to obtain the dynamical effective potential $\tilde{V}$ and the function $U$. We will use the solutions obtained in Section III in order to compute these parameters and then solve the appropriate Effective Equation of Motion (EEOM).

#### A. The dynamical effective potentials

In part I we introduced the notion of the dynamical effective potential $\tilde{V}$:

$$\tilde{V}_\chi(k=0,\chi)$$

As the fRG guarantees that the fully effective potential $V$ will be convex this implies that the dynamical effective potential $\tilde{V}$ will also be either fully or extremely close to fully convex for LPA and WFR respectively thus greatly simplifying dynamical calculations. In the previous section we emphasised how the fRG LPA effective potential gives us the Boltzmann equilibrium quantities such as equilibrium position and variance. However, away from the minimum of the effective potential the fRG gives us information that the near equilibrium Boltzmann assumption does not. To be concrete the (Gaussian) Boltzmann distribution assumes that the potential is of the form:

$$\tilde{V}_{Boltz}(x) = \frac{\gamma}{4 \cdot Var_{eq} (\chi_{eq})^2}$$

where $\chi_{eq}$ and $Var_{eq}$ are the equilibrium position and variance respectively. We show in Fig. 14 how this approximation can break down dramatically as one moves away from the equilibrium position suggesting that the fRG captures well the dynamics far away from equilibrium. In principle one could attempt to include higher order cumulants of the Boltzmann distribution such as skewness and kurtosis into the effective potential, however as we showed in part one the relationship between these cumulants and higher derivatives of the effective potential 10

### Table III: Value of the autocorrelation decay rate obtained for various potentials at different temperatures by different methods. The LPA & WFR columns display $\lambda/2$ as calculated from the fRG flow. The simulation values were generated by averaging over 10,000 runs.

| Potentials | $\Upsilon$ | LPA | WFR | Sim | $E_1$/2 |
|------------|------------|-----|-----|-----|---------|
| Poly       | 10         | 1.5929 | 1.4541 | 1.5041 | 1.4441 |
|            | 2          | 0.8484 | 0.7164 | 0.7465 | 0.6818 |
|            | 1          | 0.8557 | 0.6701 | 0.6952 | 0.5866 |
| Doublewell | 10         | 1.1262 | 0.9429 | 0.9940 | 0.9459 |
|            | 2          | 0.3002 | 0.1727 | 0.1994 | 0.1872 |
|            | 1          | 0.1467 | 0.03884 | 0.06029 | 0.05682 |
| Unequal L-J|x2 + 2 bumps| 10   | 1.4828 | 0.7767 | 0.9890 |
|            | x² + 2 bumps| 10   | 0.9705 | 0.9590 | 0.9322 |
|            | 1          | 0.9705 | 0.9590 | 0.9322 | 0.9960 |
|            | 1          | 1.6088 | 1.1149 | 1.4245 | 0.7232 |
|            | x² + 6 b/d | 2    | 0.9096 | 0.3888 | 0.4724 |
|            |            | 3    | 0.9096 | 0.3888 | 0.4724 |
FIG. 14: Comparison of $\tilde{V}$ for ULJ potential at $\Upsilon = 10$ as calculated using fRG methods LPA and WFR compared to the Boltzmann “near-equilibrium” approximation given by equation (30). All potentials have been vertically shifted so that their minima (corresponding to the equilibrium position) coincide.

potentials is highly non-trivial and is cumbersome to include.

In Fig. 15 we show the evolution of $\tilde{V}$ as $k$ is lowered to zero – or equivalently as all the fluctuations are integrated out – for the asymmetric doublewell. We can see for both the LPA (top plot) and WFR (bottom plot) how the barrier gets smaller as fluctuations are integrated out until it completely disappears. The equilibrium position is represented by the global minimum of the red curve ($k = 0$) and we can infer the speed of the evolution to this equilibrium by the slope of the curve to it. Similar behaviour can be seen for all the other potentials we consider in this paper. The fact that the fully flowed potential (red curve) is guaranteed to be (near) convex by definition of the EA $\Gamma$ ensures that the dynamics we perform in it will be trivial to solve. This is what we cover in the following subsection.

Where possible we will compare our results with those obtained by direct simulation of the Langevin equation (1) and by solving the Fokker-Plank (F-P) equation:

$$\frac{\Upsilon}{2} \frac{\partial \tilde{P}(x, t)}{\partial t} = \left( \frac{\Upsilon}{2} \right)^2 \frac{\partial^2 \tilde{P}(x, t)}{\partial x^2} + U \tilde{P}(x, t) \quad (31)$$

B. Accelerated trajectories

From part I we know that the EEOM for average position is given by:

$$\dot{\chi} = -\tilde{V}_\lambda(\chi) \quad (32)$$

Having solved the appropriate flow equations to obtain the dynamical effective potentials we can now perform dynamics in this effective potential. Given the dynamical effective potential $\tilde{V}$ it only takes a couple of seconds to obtain the full trajectory of $\chi$ from some initial position $x_i = \chi_i$, to the equilibrium position. For the polynomial potential we initialised the particle far away from the equilibrium position at $x = 4$. In Fig. 16 we show how the average position of the particle changes with time using direct simulation of the Langevin equation (1) over 5000 runs, by numerically solving the F-P equation (31) and as calculated by the evolution in the dynamical effective potentials $\tilde{V}$ given using the LPA and WFR methods at $\Upsilon = 10$. All four trajectories agree to a very high precision. This is perhaps not surprising as the polynomial potential we consider is rather simple. What is more significant however is how well the fRG works for the symmetric doublewell. In Fig. 17 we plot the four trajectories where the particle for each starts at the bottom of the right hand well ($x = \sqrt{2}$). Even the
FIG. 16: The trajectory of the average position $\chi$ in a polynomial potential $\tilde{V}$ by direct simulation & solving the EEOM [32] using LPA and WFR for $\Upsilon = 10$

FIG. 17: The trajectory of the average position $\chi$ in a doublewell potential $\tilde{V}$ by direct simulation & solving the EEOM [32] using LPA and WFR for $\Upsilon = 10$

FIG. 18: The trajectory of the average position $\chi$ in a ULJ potential $\tilde{V}$ by direct simulation & solving the EEOM [32] using LPA and WFR for $\Upsilon = 10$

FIG. 19: The trajectory of the average position $\chi$ for $x^2$ potential plus two gaussian bumps $\tilde{V}$ by direct simulation & solving the EEOM [32] using LPA and WFR for $\Upsilon = 2$. The average position $\chi$ predicted for a simple $x^2$ potential is displayed to highlight the non-trivial behaviour the fRG is capturing where competing methods struggle. Similarly in Fig. 19 the particle is initialised to the left of one of the gaussian bumps at $x = -1.5$. While the LPA offers little/no improvement over the evolution in the bare $x^2$ potential, including WFR offers excellent agreement with direct simulations and the F-P solution. This ability of the fRG to capture the non-trivial evolution of average position is also shown in Fig. 20 for the $x^2$ potential plus 6 bumps/dips which is a much more complex potential landscape. Here the LPA trajectory offers improvement over the evolution in the bare $x^2$ potential by converging to the correct equilibrium position and including WFR more closely matches the true simulated trajectory. It

simple LPA describes pretty well the evolution of $\chi(t)$ towards the equilibrium point at $\chi_{eq} = 0$. When WFR is also included it matches the simulated trajectory very closely although not quite as closely as solving the F-P equation [31]. This is a non-trivial system and it is remarkable how well the fRG does to capture the correct dynamics.

In Fig. 18 we plot the evolution of $\chi(t)$ for the ULJ potential where the particle begins in the smaller well at $x = -1.878$ and moves towards its equilibrium position. We see as before that the LPA and WFR trajectories closely match the simulated trajectory in this case bounding it above and below. For this system it was impossible to get convergent numerics for the evolution of the F-P equation [31] showing that the fRG can derive important quantities even in highly non-trivial systems.
The trajectory of the average position $\chi$ for $x^2$ potential plus 6 gaussian bumps/dips $\tilde{V}$ by direct simulation & solving the EEOM (32) using LPA and WFR for $\Upsilon = 3$ is noteworthy that the fRG is able to reasonably capture these difficult dynamics well – with significant time gains – in systems where the F-P solution is difficult to obtain.

It is important to note the time advantage offered by the fRG compared to direct numerical simulation or by solving the F-P equation \(\text{(31)}\). For example if we consider the symmetric doublewell at $\Upsilon = 10$ it takes $\sim 15$ hours to obtain good enough statistics whereas the solving the LPA flow equation takes $\sim 5$ minutes on the same machine. Including WFR is comparable to solving the F-P equation in terms of timescale at $\sim 1$ hour. Another huge advantage of the fRG is that once the dynamical effective potential $\tilde{V}$ is obtained it is trivial to solve the EEOM (32) in a couple of seconds for any initial position whereas for both direct numerical simulation of (1) and solving the F-P equation (31) one has to start again from scratch.

\section*{C. Evolution of \textbf{Var}(x)}

For our accelerated trajectories we initialised the particles at the exact same point every time. This means that at $t = 0$ the probability distribution of the particles had zero variance $\text{Var}(x) = 0$. Using this as our initial condition we solved numerically the EEOM for the variance derived in part one:

\begin{equation}
\text{Var}(x) = \frac{\Upsilon}{2\lambda P(0)} \tilde{Y}_1(t) \tilde{Y}_2(t) + \frac{P(0)}{P(t)} \left[ G_{00} - \frac{\Upsilon}{2\lambda P(0)} \right] \tilde{Y}_2^2(t) \tag{33}
\end{equation}

In Fig. 21 we show how the variance evolves with time for the polynomial potential for $\Upsilon = 5$. We can see that the LPA closely matches the numerical and F-P evolution very closely for the first 0.5 time units before departing slightly although it still tends towards the correct equilibrium distribution.

In Fig. 22 we show how the variance evolves with time for a symmetric doublewell potential for $\Upsilon = 10$. We can see that the LPA gives us excellent agreement with the simulated and F-P evolution. Considering how quickly the LPA solution is computed compared to both the F-P and directly simulated evolution, this highlights the benefit of fRG techniques for accelerated dynamics.

Finally in Figs. 23 & 24 we show how the variance evolves with time for an unequal Lennard-Jones and an $x^2$ plus 6 gaussian bumps type potential respectively. As with the one-point function, the F-P was unable to re-
solve the statistics whereas the LPA matched well the simulated trajectory, in both cases even capturing the variance overshooting its equilibrium value. Demonstrating this is particularly significant for Fig. 24 as the bare $x^2$ evolution does not capture this behaviour and overall describes the evolution poorly, converging to the wrong equilibrium variance. This shows that the fRG can also capture non-standard evolutions of non-equilibrium systems where competing methods are either ineffective, much slower, or both.

V. SUMMARY

We presented the results of various numerical solutions to the fRG flow equations and, from these solutions, solved the Effective Equations of Motion (EEOM) both in and out of equilibrium.

We have shown that a polynomial truncation of the LPA approaches the LPA result after sufficiently many terms. However, for initial potentials which are not well approximated by a polynomial, solving the full PDE is viable and accurate. We showed that the full PDE can be solved numerically using standard techniques on a variety of potentials exhibiting barrier structures and trapping wells. We also demonstrated the accuracy of the solutions, at least around the effective potential minimum, via comparisons to results from the Boltzmann distribution. The minimum of the effective potential (arising as a solution to the LPA flow equation) determines the particle’s average equilibrium position $\chi_{eq} = \lim_{t \to \infty} \langle x(t) \rangle$, while the effective potential’s curvature at the minimum determines the equilibrium variance $\lim_{t \to \infty} \left[ \langle x^2(t) \rangle - \langle x(t) \rangle^2 \right]$. We found that the computed effective potentials to give excellent results for these quantities, implying that the flow equations can be accurately solved. Beyond these time independent quantities, the curvature of the effective potential also provides an approximation to the decay rate of the equilibrium autocorrelation function $\langle x(0) x(t) \rangle_C$ but with an error that reaches $10 - 15\%$ for the potentials we examined and for temperatures relatively high compared to the heights of the potential barriers. The LPA error increases substantially as the temperature is decreased. Inclusion of WFR improves the computation of the autocorrelation function in the corresponding cases significantly, allowing for the determination of the decay rate with an accuracy of $\sim 1 - 5\%$. However, also this improvement in accuracy gets compromised at lower temperatures $\Upsilon \approx$ height of barriers.

The above observations suggest that the accuracy with which the autocorrelation function is represented by the first and second orders in the gradient expansion, LPA + the WFR correction, generically decreases with decreasing temperature. This implies that the gradient expansion of the fRG for studying thermal fluctuations is reliable only in the range from moderate temperatures (thermal energies comparable to the barrier heights), up to the very high temperature regime (where the small local features of the potential are irrelevant anyway). In contrast, at temperatures $\Upsilon$ below the height of the barriers/depth of the wells present on the potential function, the LPA+WFR approximations to the flow equation appear to break down in their ability to predict $\langle x(0) x(t) \rangle_C$. This helps to quantify the thermal window where the fRG results are both valid and non-trivial.

We showed how the out of equilibrium evolution of $\chi$ for highly non-trivial systems, such as a symmetric doublewell or an asymmetric polynomial, can be well described by fRG techniques in a fraction of the time re-
quired by both direct numerical simulation and solving the F-P equation. By comparing the evolution of $\chi$ as predicted by the fRG in potentials based on $x^2$ plus gaussian bumps to the bare $x^2$ solution we have proved that the fRG captures non-trivial local features of the potential. In fact the fRG can still offer reasonable approximations even in systems where the F-P numerics fail to converge.

We have also shown how the fRG can closely match the out of equilibrium evolution of the variance for both polynomial and doublewell potentials even just using the LPA approximation. For an Unequal Lennard-Jones type potential the LPA variance has reasonable accuracy and still captures highly non-trivial behaviour such as the variance overshooting its equilibrium value before settling to it. This is in a system for which the F-P equation fails to be resolved.

While the fRG techniques we have outlined do not offer perfect agreement with simulations they can compute non-equilibrium evolution in a tiny fraction of the time that direct numerics takes with the LPA in particular offering results over 2 orders of magnitude quicker. Also, once the fRG computes the dynamical effective potential $V$ all the dynamics for any initial condition can be trivially computed in a couple of seconds. This means that it if one wishes to calculate, for example, the evolution of an ensemble of initial conditions the fRG offers a massive advantage over direct numerical simulation or solving the F-P equation, which would have to start a new full calculation for each initial condition.

The difficulties faced obtaining results at very low temperature may indicate that the derivative expansion is insufficient for capturing dynamics in the low temperature regime. However, such a conclusion cannot be drawn solely from the results presented in this manuscript; indeed, one should investigate whether the convergence properties of the thermal problem may be improved by using a regulator function different from the Callan-Symanzik regulator, $r_1 = k$, used here. The recent findings of [19, 20] suggest that an appropriately optimized regulator, which also excludes the regime $\omega > k$ from contributing to the flow, can ensure good convergence properties and a sizeable radius of convergence. Comparisons with [19, 20] are non-trivial because the supersymmetry of the Brownian motion problem makes the structure of the flow equations different to that of a simple scalar theory. This is an important question to be resolved however.

Anther possibility is that as the temperature is lowered, the particle ends up being trapped in one of the local minima and the relevant dynamics is more akin to an escape problem, where the Kramers escape rate formula applies, rather than motion on an effective potential. The effective action may then be fundamentally non-local and not subject to a meaningful derivative expansion. We suspect this low temperature regime would bear strong similarities to quantum tunnelling computations, involving appropriate instanton-like solutions and the appropriate functional determinants from fluctuations around them. In that case an fRG study analogous to that developed in [21–23] would apply. Study of the fRG flow equation might then allow for analytic estimates of the temporal timescales required for escape over the barriers. Examining this regime further would also be an interesting direction for future investigation.

In terms of computational effort and speed, the solution of both the LPA and WFR PDEs offer significant advantages over direct numerical simulation of the Langevin equation, averaged over enough realisations to gain accurate statistics even in the more simple case of the equilibrium limit. It would be interesting to compare with standard techniques involving the Fokker-Planck equation at equilibrium, as there are well-established ways for solving the latter, and the accuracy obtained for complicated, landscape-type potentials with many bumps and dips. Obtaining accurate spectra in such complicated, non-polynomial potentials – even at equilibrium – is not trivial. fRG methods can be systematically extended to multiple degrees of freedom and therefore may offer clear computational advantages in studying the stochastic dynamics of more than one degree of freedom, especially in field theoretical problems. These are systems where the corresponding functional Fokker-Planck equation is often numerically intractable.

Future work could examine if higher order approximations beyond the WFR offer any advantage.

Advances in the above directions may lead to progress in theoretically tackling a broad range of physical phenomena with large separation between fundamental timescales of thermal fluctuations and long emergent timescales of macroscopic change, addressing what is now a major barrier for predictive simulations across scientific and engineering disciplines including materials science [24], drug design [25], protein folding [26], and cosmology [27].

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Appendix A: Solving the WFR flow equation

Including WFR does not change the evolution or final shape of \( V_k(x) \) making it irrelevant for time independent equilibrium quantities. However, as it corrects the decay rate of the correlation function it adds one more function \( \zeta_x \) to be evolved in \( k \) even for equilibrium computations. Its evolution with \( k \) for four of the potentials is shown in Figs. 25, 26, 27 & 28. As in the main body of the text we have plotted this in units where \( x = \hat{x} \) \((2D_0 = 1/\varepsilon)\) meaning \( k \) is expressed in units of \( \varepsilon \). However unlike in the main body where this choice means we express the vertical axis for the potential in units of \( \varepsilon^2 \), \( \zeta \) is merely a redefinition of length so the two axes have the same units. At the start of the flow (blue curves) \( \zeta_x = 1 \) with a non-trivial \( \chi \) dependence developing as \( k \to 0 \), shown by the red curve. Similar to the potential, as \( k \) is lowered it takes longer for changes to happen. \( \zeta_x(x) \) at \( k = 0 \) for \( \Upsilon = 1 \) is much flatter than for \( \Upsilon = 10 \). The evolution of \( \zeta_x(x) \) with \( k \) for the unequal L-J potential is shown in Fig. 27. The behaviour is similar to the doublewell case except now it is not symmetric with a larger peak for \( x > 0 \) as one might expect considering the initial shape of \( V \). The origin of these peaks is clear for the doublewell and unequal L-J potential. In both cases they form around the local minima of the bare \( V \) potential, e.g. for the doublewell this is at \( x = \pm \sqrt{2} \) which we can see matches the peak of the red curves in Fig. 26. The structure of \( \zeta_x(x) \) is even more complicated for \( x^2 \) with two bumps as shown in Fig. 28. Interestingly highly complicated
structure appears part way through the flow (around $k = 0.01$ and $k = 0.001$ for $\Upsilon = 10$ and 1 respectively) before being smoothed out as $k \to 0$. Some of this structure still remains at $\Upsilon = 1$ around the origin for $k = 0$ as similarly observed in Figs. 25, 26 & 27. Qualitatively similar behaviour is also observed for the flow of $\zeta(x)$ for $x^2$ plus 6 gaussian bumps/dips – see Fig. 29.

It is perhaps not surprising that including the running of $\zeta$ seriously complicates the numerics of the problem, equation (5) is more complicated than (3), however the effect is significant. For example we were unable to obtain stable numerics for the evolution of $\zeta$ in the unequal L-J potential for the low temperature $\Upsilon = 1$ hence its omission. The calculations for $\zeta$ also take significantly longer than for $V_k$ alone as much smaller timesteps are required to be within acceptable numerical tolerances. As an example the calculation of $V_k$ for the unequal L-J took $\sim 5$ minutes on a simple desktop machine whereas also calculating $\zeta$ on the same machine took several hours. With more specialist numerical integrators tailor made for these equations it is conceivable that computations could be done quicker and $\zeta$ could be calculated for potentials and temperatures currently inaccessible using proprietary software. The advantage of this approach compared to competing methods is that optimising solving equation (5) is independent of the potential. We leave this to future work.

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