Stationary solutions of the Vlasov-Fokker-Planck equation: existence, characterization and phase-transition

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Abstract
In this paper, we study the set of stationary solutions of the Vlasov-Fokker-Planck (VFP) equation. This equation describes the time evolution of the probability distribution of a particle moving under the influence of a double-well potential, an interaction potential, a friction force and a stochastic force. We prove, under suitable assumptions, that the VFP equation does not have a unique stationary solution and that there exists a phase transition. Our study relies on the recent results by Tugaut and coauthors regarding the McKean-Vlasov equation.

Keywords:
Invariant measure, Vlasov-Fokker-Planck equation, McKean-Vlasov equation, stochastic processes.

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1. Introduction
1.1. The Vlasov-Fokker-Planck equation
We consider the following Vlasov-Fokker-Planck (VFP) equation,
\[ \partial_t \rho = - \text{div}_q \left( \rho \frac{p}{m} \right) + \text{div}_p \left( \rho (\nabla_q V + \nabla_q \psi * \rho + \gamma \frac{p}{m}) \right) + \gamma kT \Delta_p \rho. \tag{1} \]

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In this equation, the spatial domain is $\mathbb{R}^{2d}$ with coordinates $(q,p) \in \mathbb{R}^{d} \times \mathbb{R}^{d}$. The unknown is a time-dependent probability measure $\rho: [0,T] \to \mathcal{P}(\mathbb{R}^{2d})$. Subscripts as in $\text{div}_q$ and $\Delta_p$ indicate that the differential operators act only on those variables. The functions $V = V(q)$ and $\psi = \psi(q)$ are given. The convolution $\psi * \rho$ is defined by $(\psi * \rho)(q) = \int_{\mathbb{R}^{2d}} \psi(q-q')\rho(q',p') \, dq'\,dp'$. Finally $\gamma, k$ and $T$ are positive constants.

Equation (1) is the forward Kolmogorov equation of the following stochastic differential equation (SDE),

\begin{align*}
  dQ(t) &= P(t) \, dt, \\
  dP(t) &= -\nabla V(Q(t)) \, dt - \nabla \psi \ast \rho_t(Q(t)) \, dt - \gamma \frac{P}{m} \, dt + \sqrt{2\gamma kT} \, dW(t). \quad (2)
\end{align*}

This SDE models the movement of a particle with mass $m$ under a fixed potential $V$, an interaction potential $\psi$, a friction force (the drift term $-\gamma \frac{P}{m} \, dt$) and a stochastic forcing described by the $d$-dimensional Wiener measures $W$. In this model, $\gamma$ is the friction coefficient, $k$ is the Boltzmann constant and $T$ is the absolute temperature.

Eq. (1) and system (2) play an important role in applied sciences in particular in statistical mechanics. For instance, they are used as a simplified model for chemical reactions, or as a model for particles interacting through Coulomb, gravitational, or volume exclusion forces, see e.g., [Kra40, NPT84, BD95]. Eq. (1) (and related models) has been studied intensively in the literature by many authors from various points of view, see e.g. [Deg86, BD95, BGM10, DPZ13, DPZ14, Duo15] and references therein. In particular, invariant probabilities of Eq. (1) has been investigated in [Dre87, BGM10] (see also [Duo15]). However, in these papers, the potential $V$ is assumed to be either bounded or globally Lipschitz or convex. As a result, there is a unique stationary solution. In this paper, we show that when the potential $V$ is unbounded, non-convex and non-Lipschitz, of which a double-well potential is a typical example, non-uniqueness and phase transition can occur. Herein, we characterise the set of stationary solutions in such a case. Our study relies on the recent results by Tugaut and co-authors about the McKean-Vlasov diffusion by showing that the set of stationary solutions of the Vlasov-Fokker-Planck equation is related to that of the McKean-Vlasov equation.
1.2. Normalization

We first write (1) in dimensionless form. By setting

\[ q =: L \tilde{q}, \quad p =: \frac{mL}{\tau} \tilde{p}, \quad t =: \tau \tilde{t} \]

and

\[ V(q) =: \frac{mL^2}{\tau^2} \tilde{V}(\tilde{q}), \quad \psi(q) =: \frac{mL^2}{\tau^2} \tilde{\psi}(\tilde{q}), \quad \rho(p, q, t) =: \frac{\tau^d}{mdL^2d} \tilde{\rho}(\tilde{p}, \tilde{q}, \tilde{t}), \]

where \( L \) is the characteristic length scale, and \( \tau := \frac{mL}{\gamma} \) is the relaxation time of the particle dynamics. Then the dimensionless form of the Vlasov-Fokker-Planck equation is (after leaving out all the tilde)

\[ \partial_t \rho = - \text{div}_q \left( \rho p \right) + \text{div}_p \left( \rho (\nabla_q V + \nabla_q \psi \ast \rho + p) \right) + \varepsilon \Delta_p \rho. \quad (3) \]

where \( \varepsilon := kT \tau^2 m^{-1} L^{-2} \) is the dimensionless diffusion coefficient.

In this paper, we are interested in stationary solutions of Eq. (3), i.e., solutions of the following equation

\[ K[\rho](\rho) = 0, \quad (4) \]

where

\[ K[\mu](\rho) := - \text{div}_q \left( \rho p \right) + \text{div}_p \left( \rho (\nabla_q V + \nabla_q \psi \ast \mu + p) \right) + \varepsilon \Delta_p \rho \quad (5) \]

for given \( \mu \in L^1(\mathbb{R}^d) \). Note that for a given \( \mu \), the operator \( K[\mu](\rho) \) is linear in \( \rho \). This can be seen as a linearised operator of \( K[\rho](\rho) \). Under the assumption that \( V \) and \( \psi \) are smooths, the linearised operator is hypo-elliptic.

1.3. Organisation of the paper

The rest of the paper is organised as follows. In Section 2, we state our assumptions and provide a characterization via an implicit equation for a solution of Eq. (4). In Section 3 we present main results of the paper which prove the existence, (non-) uniqueness and phase transition properties of such stationary solutions.
2. Characterization of invariant probabilities

We now characterize solutions of Eq. (4).

First of all, we consider the following assumption:

**Assumption 1 (V-1):** $V$ is a smooth function and there exists $m \in \mathbb{N}^*$ and $C_{2m} > 0$ such that $\lim_{||x|| \to +\infty} \frac{V(x)}{||x||^m} = C_{2m}$.

**Assumption (V-2):** The equation $\nabla V(x) = 0$ admits a finite number of solution. We do not specify anything about the nature of these critical points. However, the wells will be denoted by $a_0$.

**Assumption (V-3):** $V(x) \geq C_4 ||x||^4 - C_2 ||x||^2$ for all $x \in \mathbb{R}^d$ with $C_2, C_4 > 0$. $||.||$ denotes the euclidian norm.

**Assumption (V-4):** $\lim_{||x|| \to +\infty} \text{Hess } V(x) = +\infty$ and $\text{Hess } V(x) > 0$ for all $x \notin K$ where $K$ is a compact of $\mathbb{R}^d$ which contains all the critical points of $V$.

**Assumption ($\psi$-1):** There exists an even polynomial function $G$ on $\mathbb{R}$ such that $\psi(x) = G(||x||)$. And, deg$(G) =: 2n \geq 2$.

**Assumption ($\psi$-2):** $G$ and $G''$ are convex.

**Assumption ($\psi$-3):** $G(0) = 0$.

The simplest example (most famous in the literature) is that $V(x) = x^4 - x^2$ (i.e., $V$ is a double-well potential) and $\psi = \frac{\alpha}{2} x^2$ for some $\alpha$ (i.e., $\psi$ is a quadratic interaction).

**Proposition 1.** Suppose that Assumption 1 holds. If there exists a solution $\rho_\infty \in L^1 \cap L^\infty$ of Eq. (4) then

$$\rho_\infty(q,p) = Z_\varepsilon^{-1} \exp \left[ -\frac{1}{\varepsilon} \left( \frac{p^2}{2} + V(q) + \psi * \rho_\infty(q) - \psi * \rho_\infty(0) \right) \right], \quad (6)$$

where $Z_\varepsilon$ is the normalizing constant

$$Z_\varepsilon = \int_{\mathbb{R}^{2d}} \exp \left[ -\frac{1}{\varepsilon} \left( \frac{p^2}{2} + V(q) + \psi * \rho_\infty(q) - \psi * \rho_\infty(0) \right) \right] dq dp. \quad (7)$$

Conversely any measure whose density satisfies (6) is invariant for (3).

**Proof.** The idea of the proof has appeared in [Dre87], where the authors study the Vlasov-Fokker-Planck equation but with different scaling and assumptions. The proof is divided into two steps.
Step 1. We first consider the linearised equation

\[ K(\rho) := K[\mu](\rho) = 0, \]  

(8)

where \( \mu \in L^1(\mathbb{R}^d) \) is a given. We prove the following assertion: Define

\[ A := \left\{ v : \mathbb{R}^d \to \mathbb{R} \middle| v(\cdot, p) \in C^1(\mathbb{R}^d) \forall p \in \mathbb{R}^d; v(q, \cdot) \in C^2(\mathbb{R}^d) \forall q \in \mathbb{R}^d; \text{ and} \right\}. \]

Then the linearised equation (8) has a unique solution in \( A \) given by

\[ u(q, p) := C \exp \left( -\frac{1}{\varepsilon} \left( \frac{1}{2} p^2 + V(q) + \psi * \mu(q) \right) \right), \]

(9)

where \( C \) is the normalisation constant so that \( \|u\|_1 = 1 \).

Indeed, since \( -\text{div}_q(vp + \varepsilon \nabla_p V) + \Delta_p f \in L^2 \) and \( \Delta_p f \in L^2 \), we have

\[ -\text{div}_q(vp + \varepsilon \nabla_p (v \nabla_q V + \nabla_q \psi * \mu)) \]

\[ = u^{1/2} \left[ -\text{div}_q(f p) + \text{div}_p(f (\nabla_q V + \nabla_p \psi * \mu)) \right], \]

and

\[ \text{div}_p \left( vp + \varepsilon \nabla_p v \right) = \text{div}_p \left( vp + \varepsilon \nabla_p (u u^{-1/2} f) \right) \]

\[ = \text{div}_p \left( vp + \varepsilon (u \nabla_p (u^{-1/2} f) + \nabla_p u \cdot u^{-1/2} f) \right) \]

\[ = \varepsilon \text{div}_p \left( u \nabla_p (u^{-1/2} f) \right). \]

Define \( Qf := -u^{-1/2} K(u^{1/2} f) = -u^{-1/2} K(v) \). Then from the above calculation, we get

\[ Qf = -[ -\text{div}_q(f p) + \text{div}_p(f (\nabla_q V + \nabla_p \psi * \mu)) ] - \varepsilon u^{-1/2} \text{div}_p \left( u \nabla_p (u^{-1/2} f) \right). \]
Therefore, by multiplying by \( f \) and integrating over \( \mathbb{R}^2 \), we obtain

\[
\langle Qf, f \rangle_{L^2} = \frac{1}{2} \int_{\mathbb{R}^2} \left[ \text{div}_p(pf^2) - \text{div}_p(f^2(\nabla_qV + \nabla_p\psi \ast \mu)) \right] dqdp \\
- \varepsilon \int_{\mathbb{R}^2} u^{-1/2} \text{div}_p \left( u \nabla_p(u^{-1/2}f) \right) f dqdp \\
= \frac{1}{2} \int_{\mathbb{R}^2} \left[ \text{div}_p(pf^2) - \text{div}_p(f^2(\nabla_qV + \nabla_p\psi \ast \mu)) \right] dqdp \\
- \varepsilon \int_{\mathbb{R}^2} \text{div}_p \left( u^{-1/2}[u \nabla_p(u^{-1/2}f)] \right) dqdp + \varepsilon \int_{\mathbb{R}^2} u \left( \nabla_p(u^{-1/2}f) \right)^2 dqdp \\
= \varepsilon \int_{\mathbb{R}^2} u \left( \nabla_p(u^{-1/2}f) \right)^2 dqdp.
\]

Since \( Qf = 0 \), it follows that \( \nabla_p(u^{-1/2}f) = 0 \), i.e., \( u^{-1/2}f = g(q) \) for some function \( g \). Hence \( v = u^{1/2}f = u \cdot g(q) \), and \( 0 = K(v) = -up \cdot \nabla_qg(q) \). It implies that \( \nabla_qg(q) = 0 \), i.e., \( g \) is a constant. Since \( \|v\|_1 = 1 \), we obtain that \( g = 1 \), i.e. \( v = u \). In other words, Eq. (8) has \( u \) as a unique solution in \( A \) and \( \|u\|_1 = 1 \).

**Step 2.** Suppose that \( \rho_\infty \in L^1 \cap L^\infty \) is a solution of Eq. (4). Therefore, \( \rho_\infty \) solves the equation \( L[\rho_\infty](\nu) = 0 \). According to **Step 1**, this equation has a unique solution given by

\[
\tilde{\nu} = \frac{1}{Z} \exp \left[ -\frac{1}{\varepsilon^2} \left( \frac{p^2}{2} + V(q) + \psi \ast \rho_\infty(q) - \psi \ast \rho_\infty(0) \right) \right].
\]

Hence \( \tilde{\nu} = \rho_\infty \), i.e., \( \rho_\infty \) satisfies (6). The reverse assertion is obvious. \( \square \)

3. **Main results**

In this section, we assume that Assumption 1 is fulfilled.

**Theorem 1.** We consider a measure \( \rho_\infty \) on \( \mathbb{R}^d \times \mathbb{R}^d \). It is an invariant probability for (3) if and only if \( q \mapsto \int_{\mathbb{R}^d} \rho_\infty(q,p)dp \) is an invariant probability of

\[
dX(t) = -\nabla V(Q(t)) dt - \nabla \psi \ast \mu_t(X(t)) dt + \sqrt{2\varepsilon} dW(t),
\]

(10)

**Proof.** Denote by \( \tilde{\rho}_\infty \) the first marginal of \( \rho_\infty \), i.e., \( \tilde{\rho}_\infty(q) = \int_{\mathbb{R}^d} \rho_\infty(q,p)dp \). \( \square \)
Then (6) becomes

$$\rho_\infty(q, p) = \frac{\exp \left[ -\frac{1}{\varepsilon} \left( \frac{p^2}{2} + V(q) + \psi \ast \rho_\infty(q) - \psi \ast \rho_\infty(0) \right) \right]}{\int_{\mathbb{R}^d} \exp \left[ -\frac{1}{\varepsilon} \left( \frac{p^2}{2} + V(q) + \psi \ast \rho_\infty(q) - \psi \ast \rho_\infty(0) \right) \right] dq dp}$$

$$= \frac{e^{-\frac{1}{\varepsilon} \frac{p^2}{2}} \times \exp \left[ -\frac{1}{\varepsilon} \left( V(q) + \psi \ast \rho_\infty(q) - \psi \ast \rho_\infty(0) \right) \right]}{\int_{\mathbb{R}^d} e^{-\frac{1}{\varepsilon} \frac{p^2}{2}} dp \times \int_{\mathbb{R}^d} \exp \left[ -\frac{1}{\varepsilon} \left( V(q) + \psi \ast \rho_\infty(q) - \psi \ast \rho_\infty(0) \right) \right] dq}$$

(11)

It follows that

$$\hat{\rho}_\infty(q) = \int_{\mathbb{R}^d} \rho_\infty(q, p) dp = \frac{\exp \left[ -\frac{1}{\varepsilon} \left( V(q) + \psi \ast \rho_\infty(q) - \psi \ast \rho_\infty(0) \right) \right]}{\int_{\mathbb{R}^d} \exp \left[ -\frac{1}{\varepsilon} \left( V(q) + \psi \ast \rho_\infty(q) - \psi \ast \rho_\infty(0) \right) \right] dq}.$$ 

Note that $\hat{\rho}_\infty$ is the stationary measure of the McKean-Vlasov SDE

$$dX(t) = -\nabla V(Q(t)) dt - \nabla \psi \ast \mu_t(X(t)) dt + \sqrt{2\varepsilon} dW(t), \quad (12)$$

where $\mu_t$ is the law of $X(t)$. The forward Kolmogorov equation associated to the McKean-Vlasov SDE is given by

$$\partial_t \mu_t = \text{div}[\mu_t(\nabla V + \nabla \psi \ast \mu_t)] + \varepsilon \Delta \mu_t. \quad (13)$$

Thus, the following statements hold true:

**Proposition 2.** For any $\varepsilon > 0$, there exists an invariant probability.

This is a consequence of Proposition 3.1 in [Tug14b].

**Theorem 2.** If both $V$ and $\psi$ are symmetric, there exists a symmetric invariant probability.

This is a consequence of Theorem 4.5 in [HT10a].
Proposition 3. Here, $d = 1$. We assume that the interacting potential $\psi$ is quadratic: $\psi(x) := \frac{\alpha}{2} x^2$. Let $a_0$ be a critical point of $V$ such that 

$$\alpha > 2 \sup_{x \neq a_0} \frac{V(a_0) - V(x)}{(a_0 - x)^2}. \quad (14)$$

Thus, for all $\delta \in ]0; 1[$, there exists $\varepsilon_0 > 0$ such that for all $\varepsilon \leq \varepsilon_0$, Diffusion (3) admits an invariant probability $\rho_\infty$ satisfying

$$\left| \int \int q \rho_\infty(q,p) dqd\rho - a_0 + \frac{V^{(3)}(a_0)}{4V''(a_0)(\alpha + V''(a_0))} \varepsilon \right| \leq \delta \varepsilon .$$

This is a consequence of Proposition 1.2 in [Tug14a].

Theorem 3. Here, $d = 1$. We assume that 

$$V(x) = -\frac{|V''(0)|}{2} x^2 + \sum_{p=2}^q \frac{|V^{(2p)}(0)|}{(2p)!} x^{2p} \text{ with } \deg(V) =: 2q. \quad (15)$$

And, $\psi(x) := \frac{\alpha}{2} x^2$.

Thus, there exists a $\varepsilon_c > 0$ such that:

- For all $\varepsilon \geq \varepsilon_c$, Diffusion (3) admits a unique invariant probability, which is symmetric.

- For all $\varepsilon < \varepsilon_c$, Diffusion (3) admits exactly three invariant probabilities.

Moreover, $\varepsilon_c$ is the unique solution of the equation

$$\int_{\mathbb{R}^+} \left( 4y^2 - \frac{1}{2\alpha} \right) e^{(-|V''(0)|-\alpha)4y^2 - \sum_{p=2}^q \frac{2x^{p-1} |V^{(2p)}(0)|}{(2p)!} 2^{2p} y^{2p}} dy = 0. \quad (16)$$

This is a consequence of Theorem 2.1 in [Tug14a].

Proposition 4. Here, $d = 1$. We assume that $\psi$ is quadratic: $\psi(x) := \frac{\alpha}{2} x^2$. Thus, for any $\alpha \geq 0$, there exists a critical value $\varepsilon_0(\alpha)$ such that Diffusion (3) admits a unique invariant probability provided that $\varepsilon > \varepsilon_0(\alpha)$. 

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This is a consequence of Proposition 2.4 in [Tug14a].

**Theorem 4.** Let \(a_0\) be a point where \(V\) admits a local minimum such that

\[
V(x) + F(x - a_0) > V(a_0) \quad \text{for all} \quad x \neq a_0. \tag{17}
\]

Then, for all \(\kappa > 0\) small enough, there exists \(\varepsilon_0 > 0\) such that \(\forall \varepsilon \in ]0; \varepsilon_0[\), the diffusion (3) admits a stationary measure \(\rho_\infty\) satisfying

\[
\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} ||q - a_0||^{2n} \rho_\infty(q,p) dq dp \leq \kappa^{2n}.
\]

This is a consequence of Theorem 2.3 in [Tug14b].

More generally, all the results in [HT10a, HT10b, HT12, McK66, McK67, Tug10, Tug11, Tug14a, Tug14b] hold.

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