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Exponential decay of the free energy for discretized electro-reaction-diffusion systems

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Abstract

Our focus are electro-reaction-diffusion systems consisting of continuity equations for a finite number of species coupled with a Poisson equation. We take into account heterostructures, anisotropic materials and rather general statistical relations.

We introduce a discretization scheme (in space and fully implicit in time) using a fixed grid but for each species different Voronoi boxes which are defined with respect to the anisotropy matrix occurring in the flux term of this species. This scheme has the special property that it preserves the main features of the continuous systems, namely positivity, dissipativity and flux conservation.

For the discretized electro-reaction-diffusion system we investigate thermodynamic equilibria and prove for solutions to the evolution system the monotone and exponential decay of the free energy to its equilibrium value. The essential idea is an estimate of the free energy by the dissipation rate which is proved indirectly.

1 Model equations, notation, and assumptions

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain, $\Gamma := \partial\Omega$. We consider m electrically charged species X_i with charge numbers q_i and initial densities U_i. These species underly drift-diffusion processes and take part in chemical reactions. We assume that the free energy of the system is a sum of a chemical and an (electrostatic) interaction part, where the chemical part is a sum of 1-species free energies. This leads to state equations giving the relation between the densities u_i of the species X_i and the corresponding chemical potentials v_i of the type

$$u_i = \overline{u}_i g_i(v_i), \quad i = 1, \dots, m, \tag{1.1}$$

where the reference densities $\overline{u}_i$ may depend on the spatial position and expresses the possible heterogeneity of the system under consideration. The functions g_i reflect the underlying statistics. (In the case of Boltzmann statistics each g_i is the exponential function.) Our assumptions with respect to g_i (see (A2)) are such that all cases of practical interest are included, in particular the Fermi–Dirac statistics. Moreover, in the case where the chemical part of the free energy is a sum of 1-species free energies the inverse Hessian matrix is diagonal with its i-th component $\overline{u}_i g_i'(v_i)$.

Let v_0 denote the electrostatic potential. To describe the fluxes j_i of the species X_i we need the electrochemical potentials $\zeta_i := v_i + q_i v_0$. According to [1, 8, 16], we assume that the driving force for the flux is the antigradient of the electrochemical potential and that the flux is proportional the inverse Hessian. In the simplest case, with Boltzmann statistics and no anisotropies of the material, j_i is proportional to $-u_i \nabla \zeta_i$. In this paper we suppose that

$$j_i = -\overline{u}_i g_i'(v_i) \mathbf{S}_i(\cdot) \nabla \zeta_i, \; i = 1, \dots, m, \tag{1.2}$$

where the mobility $\mathbf{S}_i$ is a pointwise given symmetric positive definite matrix function which prescribes the anisotropy of the material.

To describe chemical reactions we assume that $\mathcal{R} \subset \mathbb{Z}_+^m \times \mathbb{Z}_+^m$ is a finite subset. A pair $(\alpha, \beta) \in \mathcal{R}$ represents the vectors of stoichiometric coefficients of reversible reactions, usually written in the following form:

$$\alpha_1 X_1 + \cdots + \alpha_m X_m \rightleftharpoons \beta_1 X_1 + \cdots + \beta_m X_m.$$

We assume that the net rate of this pair of reactions is of the form $k_{\alpha\beta}(a^\alpha - a^\beta)$, where $k_{\alpha\beta}$ is a reaction coefficient, $a_i := \exp(\zeta_i)$ is the electrochemical activity of X_i, and $a^\alpha := \prod_{i=1}^m a_i^{\alpha_i}$. In this model we replaced the concentrations by activities. This is necessary for the model to be in accordance with the Second Law of Thermodynamics (cf. Othmer [15]). The net production rate of species X_i corresponding to the reaction rates for all reactions taking place is

$$R_i := \sum_{(\alpha,\beta)\in\mathcal{R}} k_{\alpha\beta}(a^\alpha - a^\beta)(\beta_i - \alpha_i). \tag{1.3}$$

The continuity equation for the concentrations taking into account reaction, diffusion, and drift processes can be written as follows:

$$\begin{gathered} \frac{\partial u_i}{\partial t} + \nabla \cdot j_i = R_i \text{ in } \mathbb{R}_+ \times \Omega, \quad \nu \cdot j_i = 0 \text{ on } \mathbb{R}_+ \times \Gamma, \\ u_i(0) = U_i \text{ in } \Omega, \quad i = 1, \ldots, m. \end{gathered} \tag{1.4}$$

The Poisson equation satisfied by the electrostatic potential has the form

$$-\nabla \cdot (\mathbf{S}_0 \nabla v_0) = f + \sum_{i=1}^m q_i u_i \quad \text{in } \mathbb{R}_+ \times \Omega, \quad \nu \cdot (\mathbf{S}_0 v_0) + \tau v_0 = f^\Gamma \quad \text{on } \mathbb{R}_+ \times \Gamma, \tag{1.5}$$

with a symmetric positive definite dielectric permittivity matrix function $\mathbf{S}_0$.

Now we collect assumptions which we suppose to be fulfilled in the paper.

(A1) Ω is a bounded Lipschitzian domain in $\mathbb{R}^2$, $\Gamma = \partial\Omega$;

(A2) $g_i \in C^1(\mathbb{R}),\ \lim_{y\to\infty} \frac{1}{y} g_i(y) = +\infty,\ 0 < \delta \min\{1, g_i(y)\} \le g_i'(y) \le \delta^{-1} g_i(y),$

$\delta \min\{1, \exp(y)\} \le g_i(y) \le \delta^{-1} \exp(y),\ y \in \mathbb{R},\ i = 1, \ldots, m,$

$\overline{u}_i \in L_+^\infty(\Omega),\ \overline{u}_i \ge \delta,\ \ i = 1, \ldots, m;$

(A3) $\mathbf{S}_i \in L_+^\infty(\Omega, \mathbb{R}^{2\times 2})$ symmetric and positive definite (uniformly w.r.t. x) $i = 1, \ldots, m$;

(A4) $\mathcal{R} \subset \mathbb{Z}_+^m \times \mathbb{Z}_+^m$ finite subset, $k_{\alpha\beta} \in L_+^\infty(\Omega),\ \int_\Omega k_{\alpha\beta}\, \mathrm{d}x > 0$ for all $(\alpha, \beta) \in \mathcal{R}$;

(A5) $U_i \in L_+^\infty(\Omega),\ q_i \in \mathbb{Z},\ i = 1, \ldots, m;$

(A6) $\mathbf{S}_0 \in L_+^\infty(\Omega, \mathbb{R}^{2\times 2})$ symmetric and positive definite (uniformly w.r.t. x), $\tau \in L_+^\infty(\Gamma),\ \int_\Gamma \tau\, \mathrm{d}\Gamma > 0,\ f \in L^\infty(\Omega),\ f^\Gamma \in L^\infty(\Gamma).$

Existence results for special realizations of the electro-reaction-diffusion system (1.4), (1.5) (no anisotropies, fluxes not necessarily related to the inverse Hessian of the free energy, special statistics, restrictions concerning the reaction terms) in the sense of weak solutions can be found in [6, 7, 13]. In this paper we are interested in energy estimates for a (time and space) discrete version of (1.4), (1.5). For the continuous problem in special situations we have already obtained such results (see [11] and [9, 12] (Boltzmann statistics only)). The monotone and exponential decay of the free energy of weak solutions to (1.4), (1.5) in the setting prescribed in Section 1 is proved in [10]. There is also obtained a first result for a (time and space) discretized version of (1.4), (1.5). There is introduced a discretization scheme and its dissipativity is shown. The present paper continues the investigations in [10]. Section 2 gives a short overview on the notation, operators, energy functionals and results for the continuous problem such that analogies for the discrete version of (1.4), (1.5) can be found. Section 3 is the heart of the paper and contains the energy estimates for the discretized problem. Finally, in Section 4 we collect some remarks concerning the numerical treatment of heterostructures.

2 Continuous electro-reaction-diffusion systems

2.1 Weak formulation

To give a weak formulation of the equations (1.4), (1.5) we introduce the following spaces:

$$V := H^1(\Omega;\mathbb{R}^{m+1}),\;\; W := \{v \in V :\, \exp(v_i) \in L^\infty(\Omega),\, i = 1,\dots,m\}\,,$$

and the stoichiometric subspaces

$$\mathcal{S} := \operatorname{span}\{\alpha-\beta : (\alpha,\beta)\in\mathcal{R}\},\;\; \mathcal{S}^\perp := \text{orthogonal complement of } \mathcal{S} \text{ in } \mathbb{R}^m.$$

In addition to (A1) – (A6) we assume that we are given $U \in V^*$ such that

$$\text{(A7)}\qquad U = \Big(\sum_{i=1}^m q_i U_i, U_1,\dots,U_m\Big),\;\; \sum_{i=1}^m \lambda_i\langle U_i, 1\rangle > 0 \text{ if } \lambda = (\lambda_1,\dots,\lambda_m) \in \mathcal{S}^\perp_+\backslash\{0\}.$$

V^* denotes the space dual to V, and 1 means the constant function on Ω taking the value 1. Note that (A7) with respect to U is satisfied if $U_i \geq 0$, $U_i \neq 0$, $i = 1,\dots,m$. The element U represents an initial value for the vector function $u := (u_0,\dots,u_m)$, where

$$u_0 = \sum_{i=1}^m q_i u_i \tag{2.1}$$

is the variable charge density. We define operators $A : W \to V^*$, and $E : V \to V^*$ by

$$\begin{aligned}\langle Av, \widehat{v}\rangle := &\int_\Omega \sum_{i=1}^m \overline{u}_i g_i'(v_i)\,\mathbf{S_i}\nabla\zeta_i\cdot\nabla\widehat{\zeta}_i\,\mathrm{d}x\\ &+\int_\Omega \sum_{(\alpha,\beta)\in\mathcal{R}} k_{\alpha\beta}(a^\alpha - a^\beta)(\alpha-\beta)\cdot\widehat{\zeta}\,\mathrm{d}x,\quad v\in W,\,\widehat{v}\in V,\end{aligned}$$

where $a := (\exp(\zeta_1), \dots, \exp(\zeta_m))$, $\zeta_i = v_i + q_i v_0$, $\widehat{\zeta_i} = \widehat{v}_i + q_i \widehat{v}_0$, $i = 1, \dots, m$,

$$Ev := \big(E_0 v_0, \overline{u}_1 g_1(v_1), \dots, \overline{u}_m g_m(v_m)\big), \quad v \in V, \tag{2.2}$$

$$\langle E_0 v_0, \widehat{v}_0 \rangle := \int_\Omega \big(\mathbf{S}_0 \nabla v_0 \cdot \nabla \widehat{v}_0 - f \widehat{v}_0\big) \mathrm{d}x + \int_\Gamma \big(\tau v_0 - f^\Gamma\big) \widehat{v}_0 \, \mathrm{d}\Gamma, \quad v_0,\, \widehat{v}_0 \in H^1(\Omega).$$

A weak formulation of the transient problem (1.4), (1.5) with (1.1), (1.2), (1.3) is given by

$$\left.\begin{aligned} & u'(t) + Av(t) = 0,\ u(t) = Ev(t) \text{ f.a.a. } t \in \mathbb{R}_+,\ u(0) = U, \\ & u \in H^1_{\mathrm{loc}}(\mathbb{R}_+; V^*),\ v \in L^2_{\mathrm{loc}}(\mathbb{R}_+; V) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+; W). \end{aligned}\right\} \tag{P}$$

The dissipation rate corresponding to Problem (P), $D(v) := \langle Av, v \rangle$, $v \in W$, is nonnegative and has the form

$$D(v) = \int_\Omega \sum_{i=1}^m \overline{u}_i g_i'(v_i)\, \mathbf{S}_i \nabla \zeta_i \cdot \nabla \zeta_i \, \mathrm{d}x + \int_\Omega \sum_{(\alpha,\beta) \in \mathcal{R}} k_{\alpha\beta} (e^{\zeta\cdot\alpha} - e^{\zeta\cdot\beta})(\alpha - \beta) \cdot \zeta \mathrm{d}x.$$

To define the free energy of a state of the system under consideration we first introduce a functional $G : V \to \mathbb{R}$ as follows:

$$\begin{aligned} G(v) := & \int_\Omega \big(\frac{1}{2} \mathbf{S}_0 \nabla v_0 \cdot \nabla v_0 - f v_0\big) \, \mathrm{d}x + \int_\Gamma \big(\frac{\tau}{2} v_0^2 - f^\Gamma v_0\big) \, \mathrm{d}\Gamma \\ & + \int_\Omega \sum_{i=1}^m \int_0^{v_i} \overline{u}_i g_i(y) \, \mathrm{d}y \, \mathrm{d}x. \end{aligned} \tag{2.3}$$

The functional G is continuous, strictly convex and Gâteaux differentiable, hence subdifferentiable and $\partial G = E$. The conjugate of the functional G is denoted by F,

$$F(u) := \sup_{v \in V} \big\{\langle u, v \rangle - G(v)\big\}. \tag{2.4}$$

F is proper, lower semicontinuous and convex. Additionally, it holds $u = Ev = \partial G(v)$ if and only if $v \in \partial F(u)$. For $u \in V^*$ the value $F(u)$ is to be interpreted as the free energy of the state u. For $u \in H^1(\Omega)^* \times L^2_+(\Omega)^m$ we have

$$F(u) = \int_\Omega \sum_{i=1}^m \overline{u}_i \int_{g_i(0)}^{u_i/\overline{u}_i} g_i^{-1}(w) \, \mathrm{d}w \, \mathrm{d}x + \int_\Omega \frac{1}{2} \mathbf{S}_0 \nabla v_0 \cdot \nabla v_0 \, \mathrm{d}x + \int_\Gamma \frac{\tau}{2} v_0^2 \, \mathrm{d}\Gamma,$$

where $u_0 = E_0 v_0$. The first summand represents the chemical part of the free energy which is the sum of 1-species free energies. The last two terms give the electrostatic interaction part. Moreover, we define the subspace

$$\mathcal{U} := \Big\{ u \in V^* :\ u_0 = \sum_{i=1}^m q_i u_i,\ (\langle u_1, 1 \rangle, \dots, \langle u_m, 1 \rangle) \in \mathcal{S} \Big\}. \tag{2.5}$$

If (u, v) is a solution to (P) then $u(t) - U \in \mathcal{U}$ for every $t > 0$. Therefore, if $u^* := \lim_{t\to\infty} u(t)$ exists, then we have necessarily $u^* \in U + \mathcal{U}$. The set $\mathcal{U}^\perp := \{v \in V : \langle u, v \rangle = 0 \quad \forall u \in \mathcal{U}\}$ can be characterized as follows:

$$\mathcal{U}^\perp = \Big\{ v \in V :\ \nabla \zeta = 0,\ \zeta_i = v_i + q_i v_0,\ \zeta = (\zeta_1, \dots, \zeta_m) \in \mathcal{S}^\perp \Big\}.$$

2.2 Summary of some earlier results

Here we collect results concerning steady states and energy estimates which we have obtained in [10, Theorem 2.1, Theorem 3.2].

Theorem 2.1 *We assume* (A1) – (A7). *Then there exists a unique solution* (u^*, v^*) *to*

$$Av^* = 0, \quad u^* := Ev^*, \quad u^* \in U + \mathcal{U}, \quad v^* \in W. \tag{S}$$

It holds $\nabla\zeta^* = 0$ *and* $\zeta^* \in \mathcal{S}^\perp$.

We define the set

$$\mathcal{M} := \{(a, v_0) \in \mathbb{R}^m_+ \times H^1(\Omega) : \ a^\alpha = a^\beta \text{ for all } (\alpha,\beta) \in \mathcal{R}, \ (E_0 v_0, u_1, \ldots, u_m) \in \mathcal{U} + U,$$
$$\text{where } u_i = \overline{u}_i g_i(\ln a_i - q_i v_0) \text{ if } a_i > 0, \ u_i = 0 \text{ else}, \ i = 1, \ldots, m\}$$

and assume

(A8) $\quad \mathcal{M} \cap (\partial\mathbb{R}^m_+ \times H^1(\Omega)) = \emptyset$.

Remark 2.1 We assume (A1) – (A6). On the one hand, if (u, v) is a solution to (S) then $(a, v_0) \in \mathcal{M}$, where $a = (\mathrm{e}^{\zeta_1}, \ldots, \mathrm{e}^{\zeta_m})$. On the other hand, if $(a, v_0) \in \mathcal{M}$ and $a_i > 0$, $i = 1, \ldots, m$, then (u, v) defined by $v_i := \ln a_i - q_i v_0$, $u_i := \overline{u}_i g_i(v_i)$, $i = 1, \ldots, m$, $u_0 := E_0 v_0$ is a steady state of (P), that is a solution to (S). If in addition (A7) and (A8) are fulfilled then $\mathcal{M} = \{(a^*, v_0^*)\}$.

Theorem 2.2 *Let* (A1) – (A8) *be fulfilled, let* (u, v) *be a solution to Problem* (P), *and let* (u^*, v^*) *be the thermodynamic equilibrium* (*cf. Theorem 2.1*). *Then the free energy along the solution* (u, v) *decays monotonously and there exists a* $\lambda > 0$ *such that*

$$F(u(t)) - F(u^*) \le e^{-\lambda t}(F(U) - F(u^*)) \quad \forall\, t \ge 0.$$

The proof of Theorem 2.2 is mainly based on a Poincaré type inequality which gives an estimate of the free energy by the dissipation rate as formulated in Lemma 2.1 (see [10, Theorem 3.1], too).

Lemma 2.1 *Let* (A1) – (A8) *be fulfilled. Moreover, let* (u^*, v^*) *be the thermodynamic equilibrium according to Theorem 2.1. Then for every* $\rho > 0$ *there exists a constant* $c_\rho > 0$ *such that*

$$F(u) - F(u^*) \le c_\rho D(v) \tag{2.6}$$

for all $v \in \mathcal{N}_\rho = \{v \in W : \ F(Ev) - F(u^*) \le \rho, \ u = Ev \in U + \mathcal{U}\}$.

Remark 2.2 The proof of the exponential decay of the free energy to its equilibrium value in [10] relys essentially on Lemma 2.1 which is validated by an indirect proof. Therefore no explicit rate of convergence is obtained. But heterostructures, anisotropies, a wide class of statistics and any final set of reversible reactions are taken into account.

There are other papers which prove for special situations an explicit rate of convergence. Gajewski and Gärtner [4] did this for the van Roosbroeck system with magnetic field. Desvillettes and Fellner [2] gave an explicit rate of convergence for a reaction-diffusion system of two species and the reaction $2X_1 \rightleftharpoons X_2$ and one invariant as well as for a system of three species, the reaction $X_1 + X_2 \rightleftharpoons X_3$ and two invariants.

3 Discretized electro-reaction-diffusion systems

3.1 Space discretization

For all our considerations in Section 3 we make the following simplifying assumptions

(A9) $\overline{u}_i = \text{const},\ i = 1, \dots, m,\ k_{\alpha\beta} = \text{const},\ (\alpha, \beta) \in \mathcal{R},\ \tau = \text{const},$

$\mathbf{S}_i$ constant, symmetric, positive definite 2×2 matrices, $i = 0, \dots, m$.

Let a Delaunay grid with M grid points $\{x^k : x^k \in \overline{\Omega}, k = 1, \dots, M\}$ be given. We use the following sets of indeces

$$\mathcal{V} := \left\{k : x^k \in \overline{\Omega}\right\}, \quad \mathcal{T} := \left\{k : x^k \in \overline{\Omega} \setminus \Omega\right\}.$$

Due to (A9) the anisotropy matrices $\mathbf{S}_i$ are invertible 2×2 matrices. For $x, y \in \overline{\Omega}$ we introduce new distances defined via the anisotropy matrices $\mathbf{S}_i$,

$$d_i(x, y) := \sqrt{(x - y)^T \mathbf{S}_i^{-1} (x - y)}, \quad i = 0, \dots, m.$$

By means of these we define anisotropic Voronoi cells for each species (see Labelle and Shewchuk [14], cf. Figure 1, too)

$$V_i^k = \left\{x \in \overline{\Omega} : d_i(x, x^k) \le d_i(x, x^l) \quad \forall l \in \mathcal{V}\right\},\ i = 0, \dots, m,\ k \in \mathcal{V}.$$

For directly neighbored points x^k and x^l we denote the (outer) normal vector on V_i^k at $\partial V_i^k \cap \partial V_i^l$ by ν_i^{kl}, $i = 0, \dots, m$. Depending on the position of the grid points and the anisotropy matrices $\mathbf{S}_i$ there is a constant $c > 0$ such that

$$\frac{1}{c} \le |V_i^k| \le c, \quad |\partial V_i^k \cap \partial V_i^l| \le c, \quad k, l \in \mathcal{V},\ i = 0, \dots, m.$$

For $k \in \mathcal{V}$ we denote by u_i^k and u_0^k the mass of the i-th species in V_i^k and the charge in V_0^k, respectively. Taking into account that the Voronoi cells can differ for the different species, the relation (2.1) has to be substituted for the discrete situation by

$$u_0^k = \sum_{i=1}^m q_i \sum_{l \in \mathcal{V}} \frac{|V_0^k \cap V_i^l|}{|V_i^l|} u_i^l. \tag{3.1}$$

Associated to the grid points we have electrostatic potentials v_0^k and chemical potentials v_i^k, $i = 1, \dots, m$. The discrete version of the state equations (1.1) then is

$$u_i^k = \overline{u}_i g_i(v_i^k) |V_i^k|, \quad k \in \mathcal{V},\ i = 1, \dots, m. \tag{3.2}$$

Electrochemical potentials ζ_i^k are determined by

$$\zeta_i^k = v_i^k + q_i \sum_{l \in \mathcal{V}} \frac{|V_0^l \cap V_i^k|}{|V_i^k|} v_0^l, \quad k \in \mathcal{V},\ i = 1, \dots, m. \tag{3.3}$$

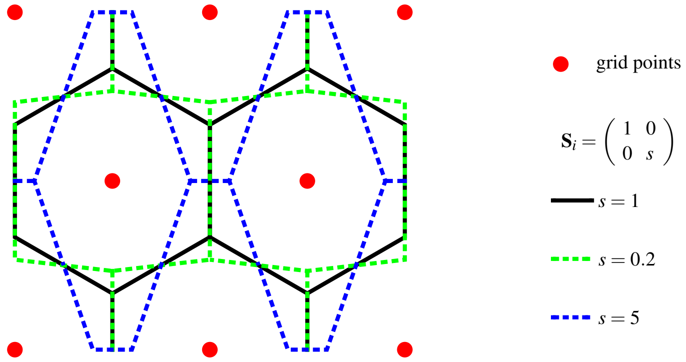

Figure 1: Different shape of anisotropic Voronoi boxes for different anisotropy matrices $\mathbf{S}_i$ for a uniform equilateral triangle mesh.

3.2 A discretization scheme for electro-reaction-diffusion systems

(A10) Let $\mathcal{Z} = \{t_0, t_1, \ldots, t_n, \ldots\}$ be a partition of $\mathbb{R}_+$ with $t_0 = 0$, $t_n \in \mathbb{R}_+$, $t_{n-1} < t_n$, $n \in \mathbb{N}$, $t_n \to +\infty$ as $n \to \infty$, $\overline{h} := \sup_{n\in\mathbb{N}}(t_n - t_{n-1}) < \infty$.

We introduce the discrete initial values

$$U_i^k := \int_{V_i^k} U_i \,\mathrm{d}x, \quad k \in \mathcal{V}, \; i = 1, \ldots, m,$$

and U_0^k is calculated via (3.1), where the u_i^l have to be substituted by U_i^l.

The space discrete version of the Poisson equation (1.5) and of the continuity equations (1.4) is obtained by testing the corresponding equations with the characteristic function of V_0^k and V_i^k, respectively, and using Gauss theorem for the divergence terms. We obtain the following discrete electro-reaction-diffusion system (PD) where the time discretization is done fully implicitly

$$\left.\begin{aligned}
&-\sum_{l\in\mathcal{V}} \frac{v_0^l(t_n) - v_0^k(t_n)}{|x^l - x^k|} |\mathbf{S}_0 \nu_0^{kl}| |\partial V_0^k \cap \partial V_0^l| + \tau v_0^k(t_n) |\partial V_0^k \cap \Gamma| - f^k = u_0^k(t_n),\\
&\frac{u_i^k(t_n) - u_i^k(t_{n-1})}{t_n - t_{n-1}} + \sum_{l\in\mathcal{V}} J_i^{kl}(t_n) |\partial V_i^k \cap \partial V_i^l| = R_i^k(t_n), \; i = 1, \ldots, m, \; n \geq 1,\\
&u_i^k(0) = U_i^k, \quad i = 0, \ldots, m, \quad k \in \mathcal{V},
\end{aligned}\right\} \quad \text{(PD)}$$

where

$$f^k = \int_{V_0^k} f \,\mathrm{d}x + \int_{\partial V_0^k \cap \Gamma} f^\Gamma \,\mathrm{d}\Gamma,$$

$$J_i^{kl}(t_n) = -\overline{u}_i \, Z_i^{kl}(t_n) \, \frac{\zeta_i^l(t_n) - \zeta_i^k(t_n)}{|x^l - x^k|} \, |\mathbf{S}_i \nu_i^{kl}|, \quad Z_i^{kl}(t_n) = \frac{g_i'(v_i^k(t_n)) + g_i'(v_i^l(t_n))}{2}.$$

The source terms R_i^k have to be calculated by

$$R_i^k(t_n) = \sum_{\alpha,\beta\in\mathcal{R}} (\beta_i - \alpha_i) \sum_{k_1\in\mathcal{V}} \cdots \sum_{k_{i-1}\in\mathcal{V}} \sum_{k_{i+1}\in\mathcal{V}} \cdots \sum_{k_m\in\mathcal{V}} R_{\alpha\beta}\big[\zeta_1^{k_1},\dots,\zeta_{i-1}^{k_{i-1}},\zeta_i^k,\zeta_{i+1}^{k_{i+1}},\dots,\zeta_m^{k_m}\big](t_n)$$
$$\times\, |V_1^{k_1}\cap\cdots\cap V_{i-1}^{k_{i-1}}\cap V_i^k\cap V_{i+1}^{k_{i+1}}\cap\cdots\cap V_m^{k_m}|$$

with

$$R_{\alpha\beta}\big[\zeta_1^{k_1},\dots,\zeta_m^{k_m}\big](t_n) = k_{\alpha\beta}\Big(\exp\Big\{\sum_{i=1}^m \alpha_i\zeta_i^{k_i}(t_n)\Big\} - \exp\Big\{\sum_{i=1}^m \beta_i\zeta_i^{k_i}(t_n)\Big\}\Big) \tag{3.4}$$

and the expression for ζ_i^k given in (3.3).

We use the notation

$$\vec u = (\vec u_0,\dots,\vec u_m),\quad \vec v = (\vec v_0,\dots,\vec v_m),\quad \vec u_i = \big(u_i^k\big)_{k\in\mathcal{V}},\quad \vec v_i = \big(v_i^k\big)_{k\in\mathcal{V}},$$
$$\vec U = (\vec U_0,\dots,\vec U_m),\quad \vec U_i = \big(U_i^k\big)_{k\in\mathcal{V}},\quad i=0,\dots,m.$$

By $\|\cdot\|$ we denote the 2-norm in $\mathbb{R}^M$ as well as in $\mathbb{R}^{M(m+1)}$, $\langle\cdot,\cdot\rangle$ means the scalar product. The discrete Poisson equation in (PD) forms a system of linear equations

$$P\vec v_0 - \vec f = \vec u_0,\quad \text{where } \vec f = \big(f^k\big)_{k=1,\dots,M}.$$

The $M\times M$ matrix P is regular, for arbitrarily given $\vec u_0$, $\vec f\in\mathbb{R}^M$ there exists a unique solution $\vec v_0\in\mathbb{R}^M$ to $P\vec v_0 - \vec f = \vec u_0$ (see [10, Lemma 4.1]). The $M\times M$ matrix P is symmetric and weakly diagonally dominant. For all $\vec y\in\mathbb{R}^M$ we have

$$\langle P\vec y,\vec y\rangle = \sum_{k,l\in\mathcal{V},\,l<k} \frac{(y^l-y^k)^2}{|x^l-x^k|}|\mathbf{S}_0\nu_0^{kl}||\partial V_0^k\cap\partial V_0^l| + \sum_{k\in\mathcal{V}}\tau\,(y^k)^2|\partial V_0^k\cap\Gamma| \ge 0. \tag{3.5}$$

Lemma 3.1 *We assume* (A1), (A6) *and* (A9). *Then there exist constants* $\gamma_1,\gamma_2>0$ *such that*

$$\gamma_1\|\vec y\|^2 \le \langle P\vec y,\vec y\rangle \le \gamma_2\|\vec y\|^2\quad \forall\vec y\in\mathbb{R}^M. \tag{3.6}$$

Proof. 1. Suppose the first inequality to be violated. Then there would exist sequences of $\vec y_n\in\mathbb{R}^M$, $c_n\in\mathbb{R}_+$, $c_n\to 0$ such that $c_n\|\vec y_n\|^2 = \langle P\vec y_n,\vec y_n\rangle$. Setting $\vec z_n := \vec y_n/\|\vec y_n\|$ we have $\langle P\vec z_n,\vec z_n\rangle = c_n\to 0$. According to (3.5) we obtain $z_n^k\to 0$ for all $k\in\mathcal{T}$. For all $\widehat k\in\mathcal{V}$ we find a finite path of neighboring Voronoi cells starting at $V_0^{\widehat k}$ and ending at a $V_0^{k^*}$, $k^*\in\mathcal{T}$, which can be used in opposite direction to show cell by cell that the corresponding $z_n^k\to 0$ and finally $z_n^{\widehat k}\to 0$, too. In summary, $\vec z_n\to 0$ in $\mathbb{R}^M$. This gives the contradiction since $\|\vec z_n\| = 1$.

2. The upper estimate follows by (3.5), (A6) and (A9). □

The discrete dissipation rate $\widehat D:\mathbb{R}^{M(m+1)}\to\mathbb{R}$ corresponding to the Problem (PD) is given by

$$\begin{aligned}\widehat D(\vec v) = &\sum_{i=1}^m \sum_{k,l\in\mathcal{V},\,l<k} \overline{u}_i\, Z_i^{kl}\frac{(\zeta_i^l-\zeta_i^k)^2}{|x^l-x^k|}|\mathbf{S}_i\nu_i^{kl}||\partial V_i^k\cap\partial V_i^l| \\ &+ \sum_{(\alpha,\beta)\in\mathcal{R}}\sum_{k_1\in\mathcal{V}}\cdots\sum_{k_m\in\mathcal{V}} R_{\alpha\beta}\big[\zeta_1^{k_1},\dots,\zeta_m^{k_m}\big]\sum_{i=1}^m(\alpha_i-\beta_i)\zeta_i^{k_i}\,|V_1^{k_1}\cap\cdots\cap V_m^{k_m}|.\end{aligned} \tag{3.7}$$

Due to (A2), (3.4) and the monotonicity of the exponential function this discrete dissipation rate is nonnegative, $\widehat{D}(\vec{v}) \geq 0$ for all $\vec{v} \in \mathbb{R}^{M(m+1)}$.

3.3 Discrete energy functionals

First, we define as a discrete version of E (cf. (2.2)) the operator $\widehat{E}\colon \mathbb{R}^{M(m+1)} \to \mathbb{R}^{M(m+1)}$,

$$\widehat{E}\vec{v} = \Big(P\vec{v}_0 - \vec{f}, \Big(\big(\overline{u}_i g_i(v_i^k)|V_i^k|\big)_{k\in\mathcal{V}}\Big)_{i=1,\dots,m}\Big).$$

The equation $\vec{u} = \widehat{E}\vec{v}$ then contains the discretized Poisson equation as well as the discrete state equations. Corresponding to $\widehat{E}$, we obtain the discrete potential $\widehat{G}\colon \mathbb{R}^{M(m+1)} \to \mathbb{R}$,

$$\widehat{G}(\vec{v}) = \frac{1}{2}\langle P\vec{v}_0, \vec{v}_0\rangle - \langle \vec{f}, \vec{v}_0\rangle + \sum_{i=1}^{m}\sum_{k\in\mathcal{V}} \overline{u}_i |V_i^k| \int_0^{v_i^k} g_i(y)\,\mathrm{d}y. \tag{3.8}$$

As in (2.3), (2.4) we introduce the discrete free energy $\widehat{F}$ as the conjugate functional,

$$\widehat{F}(\vec{u}) = \sup_{\vec{v}\in\mathbb{R}^{M(m+1)}} \big\{\langle \vec{u}, \vec{v}\rangle - \widehat{G}(\vec{v})\big\}.$$

Then $\widehat{F} : \mathbb{R}^{M(m+1)} \to \overline{\mathbb{R}}$ is convex and lower semicontinuous. $\widehat{F}$ is differentiable in arguments $\vec{u}$, where $\vec{u}_i^k > 0$, $k \in \mathcal{V}$, $i = 1,\dots,m$. If $\vec{u} = \widehat{E}\vec{v}$, then $\vec{u} = \widehat{G}'(\vec{v})$ and $\vec{v} = \widehat{F}'(\vec{u})$. In particular we obtain for $\vec{u} = \widehat{E}\vec{v}$, $\vec{v} \in \mathbb{R}^{M(m+1)}$ the inequality

$$\widehat{F}(\vec{w}) - \widehat{F}(\vec{u}) \geq \langle \vec{w} - \vec{u}, \widehat{F}'(\vec{u})\rangle \quad \forall \vec{w} \in \mathbb{R}^{M(m+1)}, \tag{3.9}$$

which is used to show that our (Euler backward in time) discretization scheme (PD) is dissipative. Moreover, for $\vec{u} = \widehat{E}\vec{v}$ we calculate

$$\begin{aligned}\widehat{F}(\vec{u}) &= \langle \widehat{E}\vec{v}, \vec{v}\rangle - \widehat{G}(\vec{v})\\ &= \frac{1}{2}\langle P\vec{v}_0, \vec{v}_0\rangle + \sum_{i=1}^{m}\sum_{k\in\mathcal{V}} \overline{u}_i |V_i^k| \Big(g_i(v_i^k)v_i^k - \int_0^{v_i^k} g_i(y)\,\mathrm{d}y\Big).\end{aligned}$$

3.4 Steady states for the discretized electro-reaction-diffusion system

In analogy to the continuous situation we define

$$\widehat{\mathcal{U}} = \Big\{\vec{u} \in \mathbb{R}^{M(m+1)} : u_0^k = \sum_{i=1}^{m} q_i \sum_{l\in\mathcal{V}} \frac{|V_0^k \cap V_i^l|}{|V_i^l|} u_i^l,\ k \in \mathcal{V},\ \big(\sum_{k\in\mathcal{V}} u_1^k, \dots, \sum_{k\in\mathcal{V}} u_m^k\big) \in \mathcal{S}\Big\}$$

and $\widehat{\mathcal{U}}^\perp = \{\vec{v} \in \mathbb{R}^{M(m+1)} : \langle \vec{u}, \vec{v}\rangle = 0 \ \ \forall \vec{u} \in \widehat{\mathcal{U}}\}$ which can be characterized by

$$\begin{aligned}\widehat{\mathcal{U}}^\perp = \Big\{\vec{v} \in \mathbb{R}^{M(m+1)} : \zeta_i^k = v_i^k + q_i \sum_{l\in\mathcal{V}} \frac{|V_0^l \cap V_i^k|}{|V_i^k|} v_0^l = \zeta_i,&\\ k \in \mathcal{V},\ i = 1,\dots,m,\ (\zeta_1,\dots,\zeta_m) \in \mathcal{S}^\perp\Big\}.&\end{aligned}$$

Lemma 3.2 *We assume* (A1) – (A6), (A9) *and* (A10). *Then*

$$\vec{u}(t_n) - \vec{U} \in \widehat{\mathcal{U}} \quad \forall n \in \mathbb{N}$$

for any solution $(\vec{u}, \vec{v})$ *to the discretized Problem* (PD).

Proof. Let $\vec{\widehat{v}} \in \widehat{\mathcal{U}}^\perp$ be arbitrarily given and $\widehat{\zeta}_i^k = \widehat{v}_i + q_i \sum_{l\in\mathcal{V}} |V_0^l \cap V_i^k||V_i^k|^{-1}\, \widehat{v}_0^l = \widehat{\zeta}_i$, $k \in \mathcal{V}$, $i = 1, \dots, m$. Then

$$\begin{aligned}
\langle \vec{u}(t_n) - \vec{U}, \vec{\widehat{v}} \rangle &= \sum_{r=1}^{n} \langle \vec{u}(t_r) - \vec{u}(t_{r-1}), \vec{\widehat{v}} \rangle = \sum_{r=1}^{n} \sum_{i=1}^{m} \sum_{k\in\mathcal{V}} \big(u_i^k(t_r) - u_i^k(t_{r-1})\big) \widehat{\zeta}_i \\
&= \sum_{r=1}^{n} \sum_{i=1}^{m} \sum_{k\in\mathcal{V}} \sum_{l\in\mathcal{V}} \overline{u}_i Z_i^{kl}(t_r) \frac{\zeta_i^l(t_r) - \zeta_i^k(t_r)}{|x^l - x^k|} |\mathbf{S}_i \nu_i^{kl}|\, \widehat{\zeta}_i\, (t_r - t_{r-1}) \\
&+ \sum_{r=1}^{n} \sum_{(\alpha,\beta)\in\mathcal{R}} \sum_{i=1}^{m} \widehat{\zeta}_i (\beta_i - \alpha_i) \sum_{k_1\in\mathcal{V}} \cdots \sum_{k_{i-1}\in\mathcal{V}} \sum_{k_i\in\mathcal{V}} \sum_{k_{i+1}\in\mathcal{V}} \cdots \sum_{k_m\in\mathcal{V}} \\
&\qquad\qquad R_{\alpha\beta}[\zeta_1^{k_1}, \dots, \zeta_m^{k_m}](t_r) |V_1^{k_1} \cap \dots \cap V_m^{k_m}| (t_r - t_{r-1}) \\
&= 0. \qquad \square
\end{aligned}$$

According to Lemma 3.2 we look for steady states $(\vec{u}, \vec{v})$ of the discretized Problem (PD) fulfilling the property $\vec{u} - \vec{U} \in \widehat{\mathcal{U}}$, and consider the problem

$$\left.\begin{aligned}
&\textstyle\sum_{l\in\mathcal{V}} J_i^{kl} |\partial V_i^k \cap \partial V_i^l| - R_i^k = 0, \ k \in \mathcal{V}, \ i = 1, \dots, m, \\
&\vec{u} = \widehat{E}\vec{v}, \quad \vec{u} - \vec{U} \in \widehat{\mathcal{U}}.
\end{aligned}\right\} \qquad \text{(SD)}$$

We introduce the functional $\widehat{G}_0 : \mathbb{R}^{M(m+1)} \to \overline{\mathbb{R}}$,

$$\widehat{G}_0(\vec{v}) := \widehat{G}(\vec{v}) + I_{\widehat{\mathcal{U}}^\perp}(\vec{v}) - \langle \vec{U}, \vec{v} \rangle, \quad \vec{v} \in \mathbb{R}^{M(m+1)},$$

where $I_{\widehat{\mathcal{U}}^\perp}$ is the characteristic function of $\widehat{\mathcal{U}}^\perp$. The functional $\widehat{G}_0$ is proper, lower semi-continuous, and strictly convex. Moreover, by the Moreau-Rockafellar theorem (see [3])

$$\partial \widehat{G}_0(\vec{v}) = \widehat{E}\vec{v} + \partial I_{\widehat{\mathcal{U}}^\perp}(\vec{v}) - \vec{U}, \quad \vec{v} \in \mathbb{R}^{M(m+1)}.$$

Lemma 3.3 *We assume* (A1) – (A7) *and* (A9). *If* $(\vec{u}, \vec{v})$ *is a solution to* (SD) *then* $\vec{v}$ *is the unique minimizer of* $\widehat{G}_0$. *On the other hand, if* $\vec{v}$ *is a minimizer of* $\widehat{G}_0$ *then* $(\widehat{E}\vec{v}, \vec{v})$ *is a solution to* (SD).

Proof. Let $(\vec{u}, \vec{v})$ be a solution to (SD). Then $\widehat{D}(\vec{v}) = 0$ and consequently $\vec{v} \in \widehat{\mathcal{U}}^\perp$. Therefore $\widehat{G}_0(\vec{v}) < \infty$ and $\partial I_{\widehat{\mathcal{U}}^\perp}(\vec{v}) = \widehat{\mathcal{U}}$. Additionally we have $\vec{u} = \widehat{E}\vec{v}$, $\vec{u} - \vec{U} = \vec{\widetilde{u}} \in \widehat{\mathcal{U}}$. Thus we find that $0 = \vec{u} - \vec{\widetilde{u}} - \vec{U} \in \partial \widehat{G}_0(\vec{v})$ which ensures that $\widehat{G}_0(\vec{v}) = \min_{\vec{w}\in\mathbb{R}^{M(m+1)}} \widehat{G}_0(\vec{w})$.

On the other hand, if $\vec{v}$ is a minimizer of $\widehat{G}_0$ then $\vec{v} \in \widehat{\mathcal{U}}^\perp$, $0 \in \partial \widehat{G}_0(\vec{v})$, and there exists $\vec{\tilde{u}} \in \partial I_{\widehat{\mathcal{U}}^\perp}(\vec{v}) = \widehat{\mathcal{U}}$ such that $\widehat{E}\vec{v} - \vec{U} = \vec{\tilde{u}} \in \widehat{\mathcal{U}}$. By $\vec{v} \in \widehat{\mathcal{U}}^\perp$ we conclude that

$$\sum_{l \in \mathcal{V}} J_i^{kl} |\partial V_i^k \cap \partial V_i^l| - R_i^k = 0, \quad k \in \mathcal{V},\ i = 1, \dots, m.$$

Thus $(\widehat{E}\vec{v}, \vec{v})$ is a solution to Problem (SD). $\square$

Theorem 3.1 *We assume* (A1) – (A7), (A9). *Then there is a unique solution* $(\vec{u}^*, \vec{v}^*)$ *to Problem* (SD). *This solution satisfies* $\vec{v}^* \in \widehat{\mathcal{U}}^\perp$.

Proof. In the proofs in this paper the letter c denotes (possibly different) constants. According to Lemma 3.3 it suffices to show that $\widehat{G}_0(\vec{v}) \to \infty$ if $\|\vec{v}\| \to \infty$. We suppose this growth condition to be violated. Then there exists $K > 0$, $\vec{v}_n \in \widehat{\mathcal{U}}^\perp$ such that $\|\vec{v}_n\| \to \infty$ and

$$\widehat{G}_0(\vec{v}_n) = \widehat{G}(\vec{v}_n) - \langle \vec{U}, \vec{v}_n \rangle \le K.$$

By the definition of $\widehat{G}$ and Lemma 3.1 this ensures

$$c\Big\{ \|\vec{v}_{n0}\|^2 + \sum_{i=1}^m \sum_{k \in \mathcal{V}} |(v_{ni}^k)^+|^2 \Big\} - \langle \vec{U}, \vec{v}_n \rangle \le K + c. \tag{3.10}$$

For $\vec{w}_n := \vec{v}_n / \|\vec{v}_n\|$ we find (for a subsequence) $\vec{w}_n \to \vec{\tilde{w}}$ in $\mathbb{R}^{M(m+1)}$ and

$$c\Big\{ \|\vec{w}_{n0}\|^2 + \sum_{i=1}^m \sum_{k \in \mathcal{V}} |(w_{ni}^k)^+|^2 \Big\} \le \frac{K + c}{\|\vec{v}_n\|^2} + \frac{\|\vec{U}\|}{\|\vec{v}_n\|}.$$

This leads to $\vec{w}_{n0} \to 0 = \vec{\tilde{w}}_0$ in $\mathbb{R}^M$, $(w_{ni}^k)^+ \to 0$ for $n \to \infty$. And $w_{ni}^k = (w_{ni}^k)^+ - (w_{ni}^k)^- \to \widetilde{w}_i^k$ ensures $-\widetilde{w}_i^k \ge 0$, $k \in \mathcal{V}$, $i = 1, \dots, m$. Since $\vec{w}_n \in \widehat{\mathcal{U}}^\perp$, $\vec{w}_n \to \vec{\tilde{w}} = (0, ((\widetilde{w}_i^k)_{k \in \mathcal{V}})_{i=1,\dots,m})$, and $\widehat{\mathcal{U}}^\perp$ is closed we find that $\vec{\tilde{w}} \in \widehat{\mathcal{U}}^\perp$, too. Therefore $\widetilde{w}_i^k = \widetilde{w}_i$, $k \in \mathcal{V}$, $i = 1, \dots, m$, and $(\widetilde{w}_1, \dots, \widetilde{w}_m) \in \mathcal{S}^\perp$. Because of $\|\vec{w}_n\| = 1$ there holds $(\widetilde{w}_1, \dots, \widetilde{w}_m) \ne 0$. We exploit again (3.10) and obtain

$$\begin{aligned} 0 = \lim_{n \to \infty} \frac{K + c}{\|\vec{v}_n\|} &\ge - \lim_{n \to \infty} \langle \vec{U}, \vec{w}_n \rangle = -\langle \vec{U}, \vec{\tilde{w}} \rangle = -\sum_{i=1}^m \sum_{k \in \mathcal{V}} U_i^k \widetilde{w}_i^k \\ &= -\sum_{i=1}^m \sum_{k \in \mathcal{V}} \int_{V_i^k} U_i \,\mathrm{d}x\ \widetilde{w}_i = -\int_\Omega \sum_{i=1}^m U_i \widetilde{w}_i \,\mathrm{d}x \end{aligned}$$

which gives a contradiction to our assumption (A7). $\square$

3.5 Energy estimates for the discretized electro-reaction-diffusion system

In [10, Theorem 4.2] we proved the dissipativity of the (fully implicit in time) discretization scheme (PD) for equidistant time steps and for a changed discretization Z_i^{kl} of the inverse

Hessian in the flux terms

$$Z_i^{kl} = \begin{cases} \frac{g_i(v_i^l)-g_i(v_i^k)}{v_i^l-v_i^k} & \text{for } v_i^l \neq v_i^k \\ g_i'(v_i^k) & \text{for } v_i^l = v_i^k \end{cases}.$$

An inspection of that proof shows that the used properties for Z_i^{kl} are that $Z_i^{kl} = Z_i^{lk} > 0$, $k, l \in \mathcal{V}$, $i = 1, \ldots, m$. In other words that result remains true for Z_i^{kl} as defined in Subsection 3.2. Our aims now are to obtain this energy estimate for arbitrary time steps (see (A10)) and especially to prove the exponential decay of the free energy as formulated for the continuous problem in Theorem 2.2 for the discretized Problem (PD), too. We start with three preparatory lemmas.

Lemma 3.4 *We assume* (A1) – (A7) *and* (A9). *Let* $\vec{u} = \widehat{E}\vec{v} \in \vec{U} + \widehat{\mathcal{U}}$ *and let* $(\vec{u}^*, \vec{v}^*)$ *be the discrete thermodynamic equilibrium according to Theorem 3.1. Then there exists a* $c > 0$ *such that*

$$\widehat{F}(\vec{u}) - \widehat{F}(\vec{u}^*) \geq c\Big\{\|\vec{v}_0 - \vec{v}_0^*\|^2 + \sum_{i=1}^m \sum_{k\in\mathcal{V}} \big|\sqrt{u_i^k} - \sqrt{u_i^{*k}}\big|^2\Big\}.$$

Proof. Using the assumptions of the lemma, $\langle \vec{u} - \vec{u}^*, \vec{v}^*\rangle = 0$ and (3.8) we evaluate

$$\begin{aligned}\widehat{F}(\vec{u}) - \widehat{F}(\vec{u}^*) &= \langle \vec{u}, \vec{v}\rangle - \widehat{G}(\vec{v}) - \langle \vec{u}^*, \vec{v}^*\rangle + \widehat{G}(\vec{v}^*) = \langle \vec{u}, \vec{v} - \vec{v}^*\rangle - \widehat{G}(\vec{v}) + \widehat{G}(\vec{v}^*) \\ &= \frac{1}{2}\langle P(\vec{v}_0 - \vec{v}_0^*), \vec{v}_0 - \vec{v}_0^*\rangle + \sum_{i=1}^m \sum_{k\in\mathcal{V}} \overline{u}_i |V_i^k| \int_{v_i^{*k}}^{v_i^k} (g_i(v_i^k) - g_i(y))\,\mathrm{d}y.\end{aligned} \tag{3.11}$$

Estimating

$$\begin{aligned}\int_{v_i^{*k}}^{v_i^k} (g_i(v_i^k) - g_i(y))\,\mathrm{d}y &\geq \delta \int_{v_i^{*k}}^{v_i^k} \Big(\frac{g_i(v_i^k)}{g_i(y)} - 1\Big) g_i'(y)\,\mathrm{d}y \\ &= \delta\Big(g_i(v_i^k)\ln\frac{g_i(v_i^k)}{g_i(v_i^{*k})} - g_i(v_i^k) + g_i(v_i^{*k})\Big) \\ &\geq \delta\Big|\sqrt{g_i(v_i^k)} - \sqrt{g_i(v_i^{*k})}\Big|^2,\end{aligned}$$

(since $x \ln\frac{x}{y} - x + y \geq (\sqrt{x} - \sqrt{y})^2$ for x, $y > 0$) we derive by (3.2) and (3.6) the desired assertion. $\square$

Lemma 3.5 *We assume* (A1) – (A7) *and* (A9). *Let* $\vec{u} = \widehat{E}\vec{v} \in \vec{U} + \widehat{\mathcal{U}}$ *and let* $(\vec{u}^*, \vec{v}^*)$ *be the thermodynamic equilibrium according to Theorem 3.1. Then there is a constant* $c > 0$ *such that*

$$\widehat{F}(\vec{u}) - \widehat{F}(\vec{u}^*) \leq c\Big\{\|\vec{v}_0 - \vec{v}_0^*\|^2 + \sum_{i=1}^m \sum_{k\in\mathcal{V}} |u_i^k - u_i^{*k}|^2\Big\}.$$

Proof. According to (3.11) and Lemma 3.1 it only remains to show that

$$\int_{v_i^{*k}}^{v_i^k} \big(g_i(v_i^k) - g_i(y)\big)\,\mathrm{d}y \le c\big(g_i(v_i^k) - g_i(v_i^{*k})\big)^2, \quad k \in \mathcal{V},\ i = 1, \dots, m.$$

Omitting the indeces k and i and having in mind that $\delta \min(1, g(y)) \le g'(y)$ (see (A2)),

$$\int_a^b \big(g(v) - g(y)\big)g'(y)\,\mathrm{d}y = g(v)\big(g(b) - g(a)\big) - \frac{1}{2}g(b)^2 + \frac{1}{2}g(a)^2,$$

$$\int_a^b \Big(\frac{g(v)}{g(y)} - 1\Big)g'(y)\,\mathrm{d}y = g(v)\ln\frac{g(b)}{g(a)} - g(b) + g(a),$$

$x \ln \frac{x}{y} - x + y \le \frac{1}{y}(x-y)^2$ for $x,\ y > 0$, and discussing the different cases for the relations between the points v, v^* and $\widetilde{v} := \arg\{g(y) = 1\}$ we find that

$$\int_{v^*}^{v} \big(g(v) - g(y)\big)\,\mathrm{d}y \le c\big(g(v) - g(v^*)\big)^2. \qquad \square$$

In analogy to the set $\mathcal{M}$ for the continuous problem, we define now the set

$$\widehat{\mathcal{M}} := \Big\{(a, \vec{v}_0) \in \mathbb{R}_+^m \times \mathbb{R}^M :\ a^\alpha = a^\beta \text{ for all } (\alpha, \beta) \in \mathcal{R},\ (P\vec{v}_0 - \vec{f}, \vec{u}_1, \dots, \vec{u}_m) \in \widehat{\mathcal{U}} + \vec{U},$$
$$\text{where } u_i^k = u_i^k(a_i, \vec{v}_0) = \overline{u}_i |V_i^k| g_i\Big(\ln a_i - q_i \sum_{l \in \mathcal{V}} \frac{|V_0^l \cap V_i^k|}{|V_i^k|} v_0^l\Big) \text{ if } a_i > 0,$$
$$u_i^k = u_i^k(a_i, \vec{v}_0) = 0 \text{ else},\ k \in \mathcal{V},\ i = 1, \dots, m\Big\}.$$

Remark 3.1 On the one hand, if $(\vec{u}, \vec{v})$ is a solution to (SD) then $(a, \vec{v}_0) \in \widehat{\mathcal{M}}$, where $a = (\mathrm{e}^{\zeta_1}, \dots, \mathrm{e}^{\zeta_m})$,

$$\zeta_i = \zeta_i^k = v_i^k + q_i \sum_{l \in \mathcal{V}} \frac{|V_0^l \cap V_i^k|}{|V_i^k|} v_0^l, \quad k \in \mathcal{V},\ i = 1, \dots, m.$$

On the other hand, if $(a, \vec{v}_0) \in \widehat{\mathcal{M}}$ and $a_i > 0$, $i = 1, \dots, m$, then $(\vec{u}, \vec{v})$ defined by $v_i^k := \ln a_i - q_i \sum_{l \in \mathcal{V}} \frac{|V_0^l \cap V_i^k|}{|V_i^k|} v_0^l$, $u_i^k := \overline{u}_i g_i(v_i^k)|V_i^k|$, $i = 1, \dots, m$, $k \in \mathcal{V}$, $\vec{u}_0 := P\vec{v}_0 - \vec{f}$, is a solution to (SD). If $\widehat{\mathcal{M}} \cap (\partial\mathbb{R}_+^m \times \mathbb{R}^M) = \emptyset$ then $\widehat{\mathcal{M}} = \{(a^*, \vec{v}_0^*)\}$.

Lemma 3.6 *Let* (A1) – (A7) *and* (A9) *be satisfied. Then*

$$\mathcal{M} \cap (\partial\mathbb{R}_+^m \times H^1(\Omega)) = \emptyset \quad \Longleftrightarrow \quad \widehat{\mathcal{M}} \cap (\partial\mathbb{R}_+^m \times \mathbb{R}^M) = \emptyset.$$

Proof. We prove here the direction $\mathcal{M} \cap (\partial\mathbb{R}_+^m \times H^1(\Omega)) = \emptyset \implies \widehat{\mathcal{M}} \cap (\partial\mathbb{R}_+^m \times \mathbb{R}^M) = \emptyset$ in great detail. At the end of the proof we give the essential hints how to show the opposite direction. The ideas then are similar to the case we discuss here. Now we show: If $\widehat{\mathcal{M}} \cap (\partial\mathbb{R}_+^m \times \mathbb{R}^M) \neq \emptyset$ then $\mathcal{M} \cap (\partial\mathbb{R}_+^m \times H^1(\Omega)) \neq \emptyset$, too. Let now be $(a, \vec{v}_0) \in \widehat{\mathcal{M}} \cap (\partial\mathbb{R}_+^m \times \mathbb{R}^M)$.

1. Case $a = 0$: Then

$$\Big(\int_\Omega U_1\,\mathrm{d}x, \ldots, \int_\Omega U_m\,\mathrm{d}x\Big) = \Big(\sum_{k\in\mathcal{V}} U_1^k, \ldots, \sum_{k\in\mathcal{V}} U_m^k\Big) \in \mathcal{S}.$$

Let $\breve{v}_0 \in H^1(\Omega)$ be the solution to $E_0\breve{v}_0 = 0$ which is uniquely defined since E_0 is strongly monotone and Lipschitz continuous. Having in mind that $U_0 = \sum_{i=1}^m q_i U_i$ we find thus that $(E_0\breve{v}_0, 0, \ldots, 0) - U \in \mathcal{U}$ and $(\breve{a}, \breve{v}_0) := (0, \breve{v}_0) \in \mathcal{M} \cap (\partial\mathbb{R}_+^m \times H^1(\Omega))$.

2. Case $a_i \neq 0$ for some $i \in \{1, \ldots, m\}$: Without loss of generality we assume that $a_i \neq 0$, $i = 1, \ldots, p$, $a_i = 0$, $i = p+1, \ldots, m$, with $1 \le p < m$. From $a^\alpha = a^\beta$ for all $(\alpha, \beta) \in \mathcal{R}$ we conclude that for all $(\alpha, \beta) \in \mathcal{R}$ with $\alpha_i > 0$ for at least one $i \in \{p+1, \ldots, m\}$ there must be at least one $\beta_j > 0$, $j \in \{p+1, \ldots, m\}$ and vice versa. Especially we have for all $(\alpha, \beta) \in \mathcal{R}$

$$\sum_{i=p+1}^m \alpha_i > 0 \Longleftrightarrow \sum_{i=p+1}^m \beta_i > 0. \tag{3.12}$$

We define

$$\widetilde{\mathcal{R}} := \Big\{(\widetilde{\alpha}, \widetilde{\beta}) = (\alpha_1, \ldots, \alpha_p, \beta_1, \ldots \beta_p) : (\alpha, \beta) \in \mathcal{R},\ \alpha_i = \beta_i = 0,\ i = p+1, \ldots, m\Big\},$$

$$\widetilde{\mathcal{S}} := \operatorname{span}\Big\{\widetilde{\alpha} - \widetilde{\beta} : (\widetilde{\alpha}, \widetilde{\beta}) \in \widetilde{\mathcal{R}}\Big\}.$$

Now we consider a dimension reduced electro-reaction-diffusion problem for the first p species with the reactions from $\widetilde{\mathcal{R}}$ and new initial values $\widetilde{U}$ which are related to the element $(a, \vec{v}_0)$ of $\widehat{\mathcal{M}} \cap (\partial\mathbb{R}_+^m \times \mathbb{R}^M)$ as follows

$$\widetilde{U} = (\widetilde{U}_0, \widetilde{U}_1, \ldots, \widetilde{U}_p), \quad \widetilde{U}_i(x) = \frac{u_i^k(a_i, \vec{v}_0)}{|V_i^k|} \text{ if } x \in V_i^k, \quad i = 1, \ldots, p, \quad \widetilde{U}_0 = \sum_{i=1}^p q_i \widetilde{U}_i.$$

We denote this problem by $(\widetilde{\mathrm{P}})$ and apply results concerning steady states from Section 2 to that problem $(\widetilde{\mathrm{P}})$. Note that for $(\widetilde{\mathrm{P}})$ the assumptions (A1) – (A7) are valid. Especially, due to the choice of $\widetilde{U}$ we have $\widetilde{U}_i > 0$, $i = 1, \ldots, p$, and the Slater condition (A7) for that dimension reduced electro-reaction-diffusion problem is fulfilled trivially. According to Theorem 2.1 there exists a unique steady state $(\widetilde{u}, \widetilde{v})$ to $(\widetilde{\mathrm{P}})$. Remark 2.1 supplies that there exists a unique $(\widetilde{a}, \widetilde{v}_0) \in \widetilde{\mathcal{M}}$,

$$\widetilde{\mathcal{M}} = \Big\{(\widetilde{a}, \widetilde{v}_0) \in \mathbb{R}_+^p \times H^1(\Omega) : \widetilde{a}^{\widetilde{\alpha}} = \widetilde{a}^{\widetilde{\beta}} \quad \forall (\widetilde{\alpha}, \widetilde{\beta}) \in \widetilde{\mathcal{R}},\ (E_0\widetilde{v}_0, \widetilde{u}_1, \ldots, \widetilde{u}_p) - \widetilde{U} \in \widetilde{\mathcal{U}},$$
$$\widetilde{u}_i = \overline{u}_i g_i(\ln \widetilde{a}_i - q_i\widetilde{v}_0) \text{ if } \widetilde{a}_i > 0,\ \widetilde{u}_i = 0 \text{ else},\ i = 1, \ldots, p\Big\}$$

with $\widetilde{a}_i > 0$, $i = 1, \ldots, p$. (Here $\widetilde{\mathcal{U}}$ is defined analogously to $\mathcal{U}$ in (2.5) substituting m by p and $\mathcal{S}$ by $\widetilde{\mathcal{S}}$.) Especially we have $E_0\widetilde{v}_0 = \sum_{i=1}^p q_i\widetilde{u}_i$ and

$$\Big(\int_\Omega (\overline{u}_1 g_1(\ln \widetilde{a}_1 - q_1\widetilde{v}_0) - \widetilde{U}_1)\,\mathrm{d}x, \ldots, \int_\Omega (\overline{u}_p g_p(\ln \widetilde{a}_p - q_p\widetilde{v}_0) - \widetilde{U}_p)\,\mathrm{d}x\Big) \in \widetilde{\mathcal{S}}. \tag{3.13}$$

Setting $(\breve a,\breve v_0) := (\widetilde a,0,\dots,0,\widetilde v_0)\in\mathbb{R}^m_+\times H^1(\Omega)$ we find $a^\alpha=a^\beta$ for all $(\alpha,\beta)\in\mathcal{R}$ (see (3.12)) and $E_0\breve v_0=\sum_{i=1}^m q_i\breve u_i$ where $\breve u_i=\widetilde u_i=\overline u_i g_i(\ln\breve a_i-q_i\breve v_0)$, $i=1,\dots,p$, $\breve u_i=0$, $i=p+1,\dots,m$. Because of

$$\int_\Omega \widetilde U_i\,\mathrm{d}x=\sum_{k\in\mathcal{V}}u_i^k(a_i,\vec v_0),\quad \int_\Omega U_i\,\mathrm{d}x=\sum_{k\in\mathcal{V}}U_i^k,$$

(3.13) and $(a,\vec v_0)\in\widehat{\mathcal{M}}\cap(\partial\mathbb{R}^m_+\times\mathbb{R}^M)$ we can verify that

$$\begin{aligned}\Big(\int_\Omega(\breve u_i-U_i)\,\mathrm{d}x\Big)_{i=1,\dots,m}&=\Big(\big(\int_\Omega(\widetilde u_i-\widetilde U_i)\,\mathrm{d}x\big)_{i=1,\dots,p},0,\dots,0\Big)\\&\quad+\Big(\big(\sum_{k\in\mathcal{V}}(u_i^k-U_i^k)\big)_{i=1,\dots,p},\big(\sum_{k\in\mathcal{V}}(0-U_i^k)\big)_{i=p+1,\dots,m}\Big)\in\mathcal{S}\end{aligned}$$

since both summands belong to $\mathcal{S}$. In summary we obtain that $(\breve a,\breve v_0)$ belongs to $\mathcal{M}\cap(\partial\mathbb{R}^m_+\times H^1(\Omega))$.

For the opposite direction one has to prove $(a,v_0)\in\mathcal{M}\cap(\partial\mathbb{R}^m_+\times H^1(\Omega))\neq\emptyset\implies\widehat{\mathcal{M}}\cap(\partial\mathbb{R}^m_+\times\mathbb{R}^M)\neq\emptyset$. The case $a=0$ is trivial. If the first p components of a are positive we have to discuss a dimension reduced discretized problem $(\widetilde{\mathrm{SD}})$ with reactions from $\widetilde{\mathcal{R}}$ and initial values

$$\vec{\widetilde U}=(\vec{\widetilde U}_0,\vec{\widetilde U}_1,\dots,\vec{\widetilde U}_p),\quad \widetilde U_i^k:=\int_{V_i^k}\overline u_i g_i(\ln a_i-q_iv_0)\,\mathrm{d}x,\quad i=1,\dots,p,$$

$$\widetilde U_0^k:=\sum_{i=1}^p q_i\sum_{l\in\mathcal{V}}\frac{|V_0^k\cap V_i^l|}{|V_i^l|}\widetilde U_i^l,\quad k\in\mathcal{V}.$$

We use results concerning steady states for the dimension reduced discretized problem from Section 3. Note that (A1) – (A6) and (A9) are fulfilled for the reduced problem. Due to

$$\int_\Omega\overline u_i g_i(\ln a_i-q_iv_0)\,\mathrm{d}x>0,\quad i=1,\dots,p,$$

(A7) is valid, too. According to Theorem 3.1 and Remark 3.1 we find a solution $(\vec{\widetilde u},\vec{\widetilde v})$ to $(\widetilde{\mathrm{SD}})$ and $(\widetilde a,\vec{\widetilde v}_0)\in\widehat{\widetilde{\mathcal{M}}}$. Then $(\breve a,\vec{\breve v}_0):=(\widetilde a,0,\dots,0,\vec{\widetilde v}_0)$ belongs to $\widehat{\mathcal{M}}\cap(\partial\mathbb{R}^m_+\times\mathbb{R}^M)$. □

In analogy to Lemma 2.1 we prove a Poincaré type inequality which gives for the discretized situation an estimate of the free energy by the dissipation rate.

Theorem 3.2 *Let* (A1) – (A9) *be fulfilled. Moreover, let* $(\vec u^*,\vec v^*)$ *be the thermodynamic equilibrium according to Theorem 3.1. Then for every* $\rho>0$ *there exists a constant* $c_\rho>0$ *such that*

$$\widehat F(\vec u)-\widehat F(\vec u^*)\le c_\rho\widehat D(\vec v)\tag{3.14}$$

for all $\vec v\in\widehat{\mathcal{N}}_\rho:=\Big\{\vec v\in\mathbb{R}^{M(m+1)}:\ \widehat F(\widehat E\vec v)-\widehat F(\vec u^*)\le\rho,\ \vec u=\widehat E\vec v\in\vec U+\widehat{\mathcal{U}}\Big\}$.

Proof. 1. Let $\rho > 0$ be arbitrarily given. For $\vec{v} \in \mathbb{R}^{M(m+1)}$, $\vec{a} = (\vec{a}_1, \dots, \vec{a}_m)$, $\vec{a}_i = \big(a_i^k\big)_{k\in\mathcal{V}}$, and $a_i^k = \exp(\zeta_i^k)$, where ζ_i^k is defined via (3.3) we can estimate

$$\begin{aligned}\widehat{D}(\vec{v}) \ge \delta \sum_{i=1}^m \sum_{k,l\in\mathcal{V},\, l<k} & Z_i^{kl} \frac{(\zeta_i^l - \zeta_i^k)^2}{|x^l - x^k|} |\partial V_i^k \cap \partial V_i^l| \\ &+ \sum_{(\alpha,\beta)\in\mathcal{R}} \sum_{k_1\in\mathcal{V}} \cdots \sum_{k_m\in\mathcal{V}} k_{\alpha\beta}\Big(\exp\Big\{\sum_{i=1}^m \zeta_i^{k_i} \frac{\alpha_i}{2}\Big\} - \exp\Big\{\sum_{i=1}^m \zeta_i^{k_i} \frac{\beta_i}{2}\Big\}\Big)^2 |V_1^{k_1} \cap \cdots \cap V_m^{k_m}| \\ &=: D_1(\vec{v}).\end{aligned}$$

Here we used (A2), (A3), (A4) and the inequality $(x-y)\ln\frac{x}{y} \ge |\sqrt{x} - \sqrt{y}|^2$ for $x, y > 0$. Therefore it suffices to prove the inequality

$$\widehat{F}(\vec{u}) - \widehat{F}(\vec{u}^*) \le C D_1(\vec{v}) \quad \forall \vec{v} \in \widehat{\mathcal{N}}_\rho. \tag{3.15}$$

2. If (3.15) would be false, then we find $\vec{v}_n \in \widehat{\mathcal{N}}_\rho$, $n \in \mathbb{N}$, such that

$$\vec{u}_n = \widehat{E}\vec{v}_n,\ \widehat{F}(\vec{u}_n) - \widehat{F}(\vec{u}^*) = C_n D_1(\vec{v}_n) > 0, \tag{3.16}$$

and $\lim_{n\to\infty} C_n = +\infty$. Let $\vec{\zeta}_n$ denote the vector of the corresponding electrochemical potentials and $a_{ni}^k = \mathrm{e}^{\zeta_{ni}^k}$ the electrochemical activities. From $\widehat{F}(\vec{u}_n) - \widehat{F}(\vec{u}^*) \le \rho$ we obtain by Lemma 3.4 that $\|\vec{u}_{ni}\| \le c$, $\|\vec{v}_{n0}\| \le c$, and by (3.2) and (A2) it results $v_{ni}^k \le c$, $0 \le a_{ni}^k \le c$, $k \in \mathcal{V}$, $i = 1, \dots, m$. In summary we find subsequences such that $a_{ni}^k \to \widehat{a}_i^k$, $k \in \mathcal{V}$, $i = 1, \dots, m$, $\vec{v}_{n0} \to \vec{\widehat{v}}_0$.

3. We write

$$(a_{ni}^k - a_{ni}^l)^2 = \Big(\frac{\mathrm{e}^{\zeta_{ni}^k} - \mathrm{e}^{\zeta_{ni}^l}}{\zeta_{ni}^k - \zeta_{ni}^l}\Big)^2 \frac{2}{g_i'(v_{ni}^k) + g_i'(v_{ni}^l)} \quad \frac{g_i'(v_{ni}^k) + g_i'(v_{ni}^l)}{2} \big(\zeta_{ni}^k - \zeta_{ni}^l\big)^2.$$

Because of $|v_{n0}^k| \le c$ and (A2) we can estimate

$$\begin{aligned}\Big(\frac{\mathrm{e}^{\zeta_{ni}^k} - \mathrm{e}^{\zeta_{ni}^l}}{\zeta_{ni}^k - \zeta_{ni}^l}\Big)^2 \frac{2}{g_i'(v_{ni}^k) + g_i'(v_{ni}^l)} &\le \mathrm{e}^{2\max\{\zeta_{ni}^k, \zeta_{ni}^l\}} \frac{2}{g_i'(\max\{v_{ni}^k, v_{ni}^l\})} \\ &\le \mathrm{e}^{c + 2\max\{v_{ni}^k, v_{ni}^l\}} \frac{2}{\delta \min\{1, g_i(\max\{v_{ni}^k, v_{ni}^l\})\}} \\ &\le \mathrm{e}^{c + 2\max\{v_{ni}^k, v_{ni}^l\}} \begin{cases} \frac{2}{\delta^2} \mathrm{e}^{-\max\{v_{ni}^k, v_{ni}^l\}} & \text{if } g_i(\max\{v_{ni}^k, v_{ni}^l\}) < 1 \\ \frac{2}{\delta} & \text{if } g_i(\max\{v_{ni}^k, v_{ni}^l\}) \ge 1 \end{cases} \le c\end{aligned}$$

since v_{ni}^k are bounded from above. Taking into account that $\frac{1}{c} \le \overline{u}_i$, $|\mathbf{S}_i \nu_i^{kl}| \le c$ we therefore conclude that

$$\sum_{k,l\in\mathcal{V},\ l<k} (a_{ni}^k - a_{ni}^l)^2 \frac{|\partial V_i^k \cap \partial V_i^l|}{|x^l - x^k|} \le c D_1(\vec{v}_n) \to 0.$$

Thus, $a_{ni}^k - a_{ni}^l \to 0$ for all k, l with $|\partial V_i^k \cap \partial V_i^l| > 0$. Using a path argument we end up with

$$a_{ni}^k \to \widehat{a}_i = \widehat{a}_i^k \quad \forall k \in \mathcal{V}, \quad i = 1, \dots, m.$$

For $(\alpha,\beta)\in\mathcal{R}$ we have

$$\prod_{i=1}^m (a_{ni}^{k_i})^{\alpha_i/2}-\prod_{i=1}^m (a_{ni}^{k_i})^{\beta_i/2}\to\prod_{i=1}^m \widehat{a}_i^{\alpha_i/2}-\prod_{i=1}^m \widehat{a}_i^{\beta_i/2}.$$

Because of

$$0\le k_{\alpha\beta}\Big(\prod_{i=1}^m (a_{ni}^{k_i})^{\alpha_i/2}-\prod_{i=1}^m (a_{ni}^{k_i})^{\beta_i/2}\Big)^2|V_1^{k_1}\cap\cdots\cap V_m^{k_m}|\le D_1(\vec{v}_n)\to 0$$

for all $k_i\in\mathcal{V}$, $i=1,\dots,m$ we have for $\widehat{a}:=(\widehat{a}_1,\dots,\widehat{a}_m)$ necessarily that

$$\widehat{a}^\alpha=\widehat{a}^\beta\quad\forall(\alpha,\beta)\in\mathcal{R}. \tag{3.17}$$

4. For $k\in\mathcal{V}$, $i=1,\dots,m$, we introduce

$$\widehat{u}_i^k:=\overline{u}_i|V_i^k|g_i\big(\ln(\widehat{a}_i)-q_i\sum_{l\in\mathcal{V}}\frac{|V_0^l\cap V_i^k|}{|V_i^k|}\widehat{v}_0^l\big)\ \text{if}\ \widehat{a}_i\ne 0,\ \ \widehat{u}_i^k:=0\ \text{if}\ \widehat{a}_i=0. \tag{3.18}$$

Due to $0<g_i'(\theta)\le\delta^{-1}g_i(\theta)\le\delta^{-2}\mathrm{e}^\theta$ the generalized mean value theorem ensures

$$\frac{|g_i(x)-g_i(y)|}{|\mathrm{e}^x-\mathrm{e}^y|}\le\sup_{\theta\in[x,y]}\frac{g_i'(\theta)}{\mathrm{e}^\theta}\le c, \tag{3.19}$$

and we can estimate for $\widehat{u}_i^k\ne 0$ that

$$\begin{aligned}|u_{ni}^k-\widehat{u}_i^k|&\le c\Big|g_i\big(\ln(a_{ni}^k)-q_i\sum_{l\in\mathcal{V}}\frac{|V_0^l\cap V_i^k|}{|V_i^k|}v_{n0}^l\big)-g_i\big(\ln(\widehat{a}_i)-q_i\sum_{l\in\mathcal{V}}\frac{|V_0^l\cap V_i^k|}{|V_i^k|}\widehat{v}_0^l\big)\Big|\\&\le c\Big|\exp\big(\ln(a_{ni}^k)-q_i\sum_{l\in\mathcal{V}}\frac{|V_0^l\cap V_i^k|}{|V_i^k|}v_{n0}^l\big)-\exp\big(\ln(\widehat{a}_i)-q_i\sum_{l\in\mathcal{V}}\frac{|V_0^l\cap V_i^k|}{|V_i^k|}\widehat{v}_0^l\big)\Big|\\&\le c\Big(|a_{ni}^k-\widehat{a}_i|+(a_{ni}^k+1)\sum_{l\in\mathcal{V}}\frac{|V_0^l\cap V_i^k|}{|V_i^k|}|v_{n0}^l-\widehat{v}_0^l|\Big)\to 0.\end{aligned}$$

Such an estimate for $|u_{ni}^k-\widehat{u}_i^k|$ is true also if $\widehat{u}_i^k=0$.

5. According to (3.1), we set $\widehat{u}_0^k:=\sum_{i=1}^m q_i\sum_{l\in\mathcal{V}}\frac{|V_0^k\cap V_i^l|}{|V_i^l|}\widehat{u}_i^l$ and $\widehat{\vec{u}}:=(\widehat{\vec{u}}_0,\widehat{\vec{u}}_1,\dots,\widehat{\vec{u}}_m)$. Because of $\vec{u}_n-\vec{U}\in\widehat{\mathcal{U}}$ we obtain $\widehat{\vec{u}}-\vec{U}\in\widehat{\mathcal{U}}$. Let $\vec{v}_0^o$ denote the solution to $P\vec{v}_0^o-\vec{f}=\widehat{\vec{u}}_0$. Since $u_{n0}^k\to\widehat{u}_0^k$ we find $P^{-1}(\vec{u}_{n0}-\widehat{\vec{u}}_0)=\vec{v}_{n0}-\vec{v}_0^o\to 0$. Together with $\vec{v}_{n0}\to\widehat{\vec{v}}_0$ this yields $\widehat{\vec{v}}_0=\vec{v}_0^o$ and $P\widehat{\vec{v}}_0-\vec{f}=\widehat{\vec{u}}_0$. Thus, $(\widehat{a},\widehat{\vec{v}}_0)\in\widehat{\mathcal{M}}$, and according to (A8) and Lemma 3.6 this is possible only if $\widehat{a}_i>0$, $i=1,\dots,m$. Defining

$$\widehat{\zeta}_i:=\ln(\widehat{a}_i),\quad \widehat{v}_i^k:=\widehat{\zeta}_i-q_i\sum_{l\in\mathcal{V}}\frac{|V_0^l\cap V_i^k|}{|V_i^k|}\widehat{v}_0^l,\ i=1,\dots,m,$$

we get $\widehat{\vec{v}}:=(\widehat{\vec{v}}_0,\widehat{\vec{v}}_1,\dots,\widehat{\vec{v}}_m)\in\mathbb{R}^{M(m+1)}$, $\widehat{\vec{u}}=\widehat{E}\widehat{\vec{v}}\in\vec{U}+\widehat{\mathcal{U}}$, and

$$\sum_{l\in\mathcal{V}}J_i^{kl}|\partial V_i^k\cap\partial V_i^l|-R_i^k=0,\quad k\in\mathcal{V},\ i=1,\dots,m.$$

Thus, $(\vec{\bar{u}},\vec{\bar{v}})$ is a solution to (SD). By Theorem 3.1 we conclude that $\vec{\bar{v}}=\vec{v}^*$ and $\vec{\bar{u}}=\vec{u}^*$.
6. Due to the convergence of the sequences $(\vec{v}_{n0})$ and $(\vec{u}_n)$ and Lemma 3.5 we have

$$\lambda_n := \sqrt{\widehat{F}(\vec{u}_n)-\widehat{F}(\vec{u}^*)} \to 0 \text{ as } n\to\infty. \tag{3.20}$$

Additionally (according to (3.16)) we find

$$\frac{1}{C_n}=\frac{1}{\lambda_n^2}D_1(\vec{v}_n)\to 0 \text{ as } n\to\infty. \tag{3.21}$$

We introduce the quantities

$$\vec{w}_{n0}:=\frac{1}{\lambda_n}(\vec{v}_{n0}-\vec{\bar{v}}_0),\quad \vec{y}_n:=\frac{1}{\lambda_n}(\vec{u}_n-\vec{\bar{u}}),\quad b_{ni}^k:=\frac{1}{\lambda_n}\Big(\sqrt{\frac{a_{ni}^k}{\widehat{a}_i}}-1\Big),\ k\in\mathcal{V},\ i=1,\dots,m.$$

The relation

$$\big(b_{ni}^k-b_{ni}^l\big)^2=\left(\frac{\sqrt{\frac{a_{ni}^k}{\widehat{a}_i}}-\sqrt{\frac{a_{ni}^l}{\widehat{a}_i}}}{\zeta_{ni}^k-\zeta_{ni}^l}\right)^2\frac{2}{g_i'(v_{ni}^k)+g_i'(v_{ni}^l)}\,\frac{g_i'(v_{ni}^k)+g_i'(v_{ni}^l)}{2}\,\frac{(\zeta_{ni}^k-\zeta_{ni}^l)^2}{\lambda_n^2}$$

and the estimate

$$\begin{aligned}&\left(\frac{\sqrt{\frac{a_{ni}^k}{\widehat{a}_i}}-\sqrt{\frac{a_{ni}^l}{\widehat{a}_i}}}{\zeta_{ni}^k-\zeta_{ni}^l}\right)^2\frac{2}{g_i'(v_{ni}^k)+g_i'(v_{ni}^l)}=\left(\frac{\exp\frac{\zeta_{ni}^k-\widehat{\zeta}_i}{2}-\exp\frac{\zeta_{ni}^l-\widehat{\zeta}_i}{2}}{\zeta_{ni}^k-\zeta_{ni}^l}\right)^2\frac{2}{g_i'(v_{ni}^k)+g_i'(v_{ni}^l)}\\
&\le\frac{1}{2\widehat{a}_i}\exp\{\max\{\zeta_{ni}^k,\zeta_{ni}^l\}\}\frac{1}{g_i'(\max\{v_{ni}^k,v_{ni}^l\})}\\
&\le c\exp\{c+\max\{v_{ni}^k,v_{ni}^l\}\}\begin{cases}\frac{1}{\delta^2}\exp\{-\max\{v_{ni}^k,v_{ni}^l\}\} & \text{if } g_i(\max\{v_{ni}^k,v_{ni}^l\})<1\\ \frac{1}{\delta} & \text{if } g_i(\max\{v_{ni}^k,v_{ni}^l\})\ge 1\end{cases}\end{aligned}$$

together with $v_{ni}^k\le c$, $k\in\mathcal{V}$ guarantee that

$$\sum_{k,l\in\mathcal{V},l<k}\big(b_{ni}^k-b_{ni}^l\big)^2\frac{|\partial V_i^k\cap\partial V_i^l|}{|x^k-x^l|}\le c\frac{D_1(\vec{v}_n)}{\lambda_n^2}\to 0.$$

Thus, $b_{ni}^k-b_{ni}^l\to 0$ for all k,l with $|\partial V_i^k\cap\partial V_i^l|>0$. By a path argument we end up with

$$b_{ni}^k\to\widehat{b}_i\quad\forall k\in\mathcal{V},\quad i=1,\dots,m.$$

Lemma 3.4 ensures that $\|\vec{w}_{n0}\|\le c$. Since

$$|y_{ni}^k|=\frac{|u_{ni}^k-\widehat{u}_i^k|}{\lambda_n}\le\big|\sqrt{u_{ni}^k}+\sqrt{\widehat{u}_i^k}\big|\frac{|\sqrt{u_{ni}^k}-\sqrt{\widehat{u}_i^k}|}{\lambda_n}$$

and $|u_{ni}^k|$, $|\widehat{u}_i^k|\le c$ (see step 2 and 4) we find by Lemma 3.4 that $\|\vec{y}_{ni}\|\le c$, $i=1,\dots,m$. Thus there are subsequences and elements $\vec{\bar{w}}_0$ and $\vec{\bar{y}}$ such that

$$\vec{w}_{n0}\to\vec{\bar{w}}_0,\quad \vec{y}_{ni}\to\vec{\bar{y}}_i,\ i=0,\dots,m.$$

7. In view of $\vec{u}_n - \vec{U} \in \widehat{\mathcal{U}}$ we have $\vec{y}_n \in \widehat{\mathcal{U}}$. Passing to the limit we find that $\vec{\widehat{y}} \in \widehat{\mathcal{U}}$, thus

$$\Big(\sum_{k\in\mathcal{V}} \widehat{y}_1^k, \dots, \sum_{k\in\mathcal{V}} \widehat{y}_m^k\Big) \in \mathcal{S}. \tag{3.22}$$

By the definition of b_{ni}^k and $\widehat{a}$ we obtain for all $(\alpha,\beta) \in \mathcal{R}$,

$$\begin{aligned}\widehat{a}^{\,-\alpha}\Big(\prod_{i=1}^m (a_{ni}^{k_i})^{\alpha_i/2} - \prod_{i=1}^m (a_{ni}^{k_i})^{\beta_i/2}\Big)^2 &= \Big(\prod_{i=1}^m (\lambda_n b_{ni}^{k_i}+1)^{\alpha_i} - \prod_{i=1}^m (\lambda_n b_{ni}^{k_i}+1)^{\beta_i}\Big)^2 \\ &= \Big(\lambda_n \sum_{i=1}^m b_{ni}^{k_i}(\alpha_i-\beta_i)\Big)^2 + Q_n(k_1,\dots,k_n)\end{aligned} \tag{3.23}$$

where

$$|Q_n(k_1,\dots,k_n)| \le c\lambda_n^3(\|b_n\|+1)^{p_0} \quad \forall k_1,\dots,k_n \in \mathcal{V},$$
$$0 \le p_0 \le 2 \max_{(\alpha,\beta)\in\mathcal{R}} \max\Big\{\sum_{i=1}^m \alpha_i, \sum_{i=1}^m \beta_i\Big\}.$$

Taking into account that $\lambda_n \to 0$ as $n\to\infty$, we find

$$\frac{1}{\lambda_n^2}|Q_n(k_1,\dots,k_n)| \le c\lambda_n(\|b_n\|+1)^{p_0} \to 0 \text{ as } n\to\infty \quad \forall k_1,\dots,k_n \in \mathcal{V}.$$

This together with (3.21) and (3.23) gives

$$\lim_{n\to\infty} \sum_{k_1\in\mathcal{V}} \cdots \sum_{k_m\in\mathcal{V}} k_{\alpha\beta}\Big(\sum_{i=1}^m b_{ni}^{k_i}(\alpha_i-\beta_i)\Big)^2 |V_1^{k_1}\cap\dots\cap V_m^{k_m}| = 0 \quad \forall (\alpha,\beta)\in\mathcal{R}.$$

Therefore, for $\widehat{b} = (\widehat{b}_1,\dots,\widehat{b}_m)$ where $\widehat{b}_i = \lim_{n\to\infty} b_{ni}^k$, $k\in\mathcal{V}$, we arrive at

$$\widehat{b} \in \mathcal{S}^\perp. \tag{3.24}$$

8. Letting $n\to\infty$ in

$$y_{ni}^k = \frac{\overline{u}_i|V_i^k|}{\lambda_n}\Big(g_i\big(\ln(a_{ni}^k) - q_i\sum_{l\in\mathcal{V}}\frac{|V_0^l\cap V_i^k|}{|V_i^k|}v_{n0}^l\big) - g_i\big(\ln(\widehat{a}_i) - q_i\sum_{l\in\mathcal{V}}\frac{|V_0^l\cap V_i^k|}{|V_i^k|}\widehat{v}_0^l\big)\Big)$$

we find

$$\begin{aligned}\widehat{y}_i^k &= \overline{u}_i|V_i^k|g_i'\big(\ln(\widehat{a}_i) - q_i\sum_{l\in\mathcal{V}}\frac{|V_0^l\cap V_i^k|}{|V_i^k|}\widehat{v}_0^l\big)\big(2\widehat{b}_i - q_i\sum_{l\in\mathcal{V}}\frac{|V_0^l\cap V_i^k|}{|V_i^k|}\widehat{w}_0^l\big) \\ &= \overline{u}_i|V_i^k|g_i'(\widehat{v}_i^k)\big(2\widehat{b}_i - q_i\sum_{l\in\mathcal{V}}\frac{|V_0^l\cap V_i^k|}{|V_i^k|}\widehat{w}_0^l\big).\end{aligned} \tag{3.25}$$

Lemma 3.1 and the equations satisfied by $\vec{v}_{n0}$ and $\vec{\widehat{v}}_0$, respectively, imply

$$c\|\vec{v}_{n0}-\vec{\widehat{v}}_0\|^2 \le \langle P(\vec{v}_{n0}-\vec{\widehat{v}}_0), \vec{v}_{n0}-\vec{\widehat{v}}_0\rangle = \sum_{i=1}^m q_i \sum_{k\in\mathcal{V}}\sum_{l\in\mathcal{V}} \frac{|V_0^k\cap V_i^l|}{|V_i^l|}(u_{ni}^l-\widehat{u}_i^l)(v_{n0}^k-\widehat{v}_0^k). \tag{3.26}$$

Dividing by λ_n^2 and passing to the limit as $n \to \infty$, we obtain

$$c\|\vec{\overline{w}}_0\|^2 \le \sum_{i=1}^m q_i \sum_{k\in\mathcal{V}} \sum_{l\in\mathcal{V}} \frac{|V_0^k \cap V_i^l|}{|V_i^l|} \widehat{y}_i^{\,l}\, \widehat{w}_0^k \,\mathrm{d}x.$$

According to (3.22), (3.24) we have $\sum_{i=1}^m \sum_{l\in\mathcal{V}} \widehat{y}_i^{\,l}\, \widehat{b}_i = 0$, and additionally using (3.25) we derive from the previous inequality

$$\begin{aligned} c\|\vec{\overline{w}}_0\|^2 &\le \sum_{i=1}^m \sum_{l\in\mathcal{V}} \widehat{y}_i^{\,l} \Big(q_i \sum_{k\in\mathcal{V}} \frac{|V_0^k \cap V_i^l|}{|V_i^l|} \widehat{w}_0^k - 2\widehat{b}_i \Big) \\ &= -\sum_{i=1}^m \sum_{l\in\mathcal{V}} \overline{u}_i |V_i^l| g_i'(\widehat{v}_i^l) \Big(q_i \sum_{k\in\mathcal{V}} \frac{|V_0^k \cap V_i^l|}{|V_i^l|} \widehat{w}_0^k - 2\widehat{b}_i \Big)^2 \le 0. \end{aligned}$$

Thus it follows $\vec{\overline{w}}_0 = 0$, $\widehat{b} = 0$, and $\vec{\overline{y}} = 0$.

9. By the definition of λ_n (see (3.20)) and Lemma 3.5 we find

$$1 = \frac{1}{\lambda_n^2} \Big(\widehat{F}(\vec{u}_n) - \widehat{F}(\vec{u}^*) \Big) \le c \Big(\|\vec{\overline{w}}_{n0}\|^2 + \sum_{i=1}^m \|\vec{\overline{y}}_{ni}\|^2 \Big).$$

Because of $\vec{\overline{w}}_{n0} \to 0$, $\vec{\overline{y}}_{ni} \to 0$ the right hand side converges to 0 as $n \to \infty$. This contradiction shows that the assumption made in the beginning of step 2 of the proof was wrong, i.e., (3.15) holds, and the proof is complete. □

Now we are able to prove the main result of the paper which concerns the (monotone and) exponential decay of the free energy on solutions to the discretized Problem (PD).

Theorem 3.3 *We assume* (A1) – (A10). *Then the* (*fully implicit in time*) *discretization scheme* (PD) *is dissipative, i.e. solutions* $(\vec{u}, \vec{v})$ *to* (PD) *fulfil*

$$\widehat{F}(\vec{u}(t_{n_2})) \le \widehat{F}(\vec{u}(t_{n_1})) \le \widehat{F}(\vec{U}) \quad \textit{for all } t_{n_1} \le t_{n_2}.$$

Moreover, there exists a $\lambda > 0$ *such that*

$$\widehat{F}(\vec{u}(t_n)) - \widehat{F}(\vec{u}^*) \le e^{-\lambda t_n} \big(\widehat{F}(\vec{U}) - \widehat{F}(\vec{u}^*) \big) \quad \forall n \ge 1.$$

Proof. 1. According to Lemma 3.2, a solution $(\vec{u}, \vec{v})$ to the discrete Problem (PD) fulfills the invariance property

$$\vec{u}(t_n) - \vec{U} \in \widehat{\mathcal{U}}, \quad n \ge 1.$$

2. $\widehat{F}$ is differentiable in arguments $\vec{u}$, where $u_i^k > 0$, $k \in \mathcal{V}$, $i = 1, \dots, m$. If $\vec{u} = \widehat{E}\vec{v}$, then $\vec{u} = \widehat{G}'(\vec{v})$ and $\vec{v} = \widehat{F}'(\vec{u})$ and we obtain the inequality

$$\widehat{F}(\vec{w}) - \widehat{F}(\vec{u}) \ge \langle \vec{v}, \vec{w} - \vec{u} \rangle \quad \forall \vec{w} \in \mathbb{R}^{M(m+1)}. \tag{3.27}$$

3. Let $n_2 > n_1 \geq 0$ and $\lambda \geq 0$. Using $\vec{u}(t_r) = \widehat{E}\vec{v}(t_r)$, (3.27), the discrete continuity equations in (PD), and the definition of the discrete dissipation rate (3.7) we estimate

$$\begin{aligned}
&\mathrm{e}^{\lambda t_{n_2}}\Big(\widehat{F}(\vec{u}(t_{n_2})) - \widehat{F}(\vec{u}^*)\Big) - \mathrm{e}^{\lambda t_{n_1}}\Big(\widehat{F}(\vec{u}(t_{n_1})) - \widehat{F}(\vec{u}^*)\Big) \\
&= \sum_{r=n_1+1}^{n_2} \Big\{(\mathrm{e}^{\lambda t_r} - \mathrm{e}^{\lambda t_{r-1}})\big(\widehat{F}(\vec{u}(t_r)) - \widehat{F}(\vec{u}^*)\big) + \mathrm{e}^{\lambda t_{r-1}}\big(\widehat{F}(\vec{u}(t_r)) - \widehat{F}(\vec{u}(t_{r-1}))\big)\Big\} \\
&\leq \sum_{r=n_1+1}^{n_2} \Big\{\mathrm{e}^{\lambda t_{r-1}}(\mathrm{e}^{\lambda(t_r - t_{r-1})} - 1)\big(\widehat{F}(\vec{u}(t_r)) - \widehat{F}(\vec{u}^*)\big) + \mathrm{e}^{\lambda t_{r-1}}\langle \vec{u}(t_r) - \vec{u}(t_{r-1}), \vec{v}(t_r)\rangle\Big\} \\
&\leq \sum_{l=n_1+1}^{n_2} \mathrm{e}^{\lambda t_{r-1}}\,(t_r - t_{r-1})\Big\{\mathrm{e}^{\lambda\overline{h}}\lambda\big(\widehat{F}(\vec{u}(t_r)) - \widehat{F}(\vec{u}^*)\big) - \widehat{D}(\vec{v}(t_r))\Big\}.
\end{aligned} \tag{3.28}$$

4. Since $\widehat{D}(\vec{v}) \geq 0$ for $\vec{v} \in \mathbb{R}^{M(m+1)}$, we obtain by setting $\lambda = 0$ in (3.28) that

$$\widehat{F}(\vec{u}(t_{n_2})) \leq \widehat{F}(\vec{u}(t_{n_1})) \leq \widehat{F}(\vec{U}) \quad \forall n_2 \geq n_1 \geq 0.$$

5. Setting $\rho := \widehat{F}(\vec{U}) - \widehat{F}(\vec{u}^*)$ we find $\widehat{F}(\vec{u}(t_r)) - \widehat{F}(\vec{u}^*) \leq \rho$, $\vec{u}(t_r) = \widehat{E}\vec{v}(t_r) \in \vec{U} + \widehat{\mathcal{U}}$. This means $\vec{v}(t_r) \in \widehat{\mathcal{N}}_\rho$ for $r \geq 1$. Theorem 3.2 supplies a $c_\rho > 0$ such that (3.14) is fulfilled. Choosing now $\lambda > 0$ such that $\lambda \mathrm{e}^{\lambda\overline{h}} c_\rho < 1$ (see (A10), too) and $n_1 = 0$, the estimate (3.28) proves the second part of the theorem. $\square$

Remark 3.2 Gajewski and Gärtner [5] use a Crank-Nicholson like time discretization to show the dissipativeness for a discrete scheme for a nonlocal phase segregation model. This there is necessary due to the fact that the free energy functional in that model is not convex. In our convex situation we can apply an Euler backward scheme because we can exploit inequality (3.27) to proceed in the proof of Theorem 3.3.

4 Remarks on the numerical treatment of heterostructures

We consider a 2D heterostructure, where in subregions the material parameters are constants and intend to apply the techniques from Section 3 to this situation in a suitable way. Let $\Omega \in \mathbb{R}^2$ be composed by a finite number of connected, bounded, nonempty polyhedral open subsets Ω^I, $I \in \mathcal{I}$, with common edges $\Gamma^{AB} = \overline{\Omega^A} \cap \overline{\Omega^B}$, $\overline{\Omega} = \cup_{I \in \mathcal{I}} \overline{\Omega^I}$. On Ω^I we assume constant material parameters $\overline{u}_i^I$, $k_{\alpha\beta}^I$, $\mathbf{S}_i^I$, $I \in \mathcal{I}$ (see (A9), too). The mobility and dielectric permittivity matrices $\mathbf{S}_i^I$ have the form

$$\mathbf{S}_i^I = Q_i^{I^T} \operatorname{diag}\,(\mu_i^{1I}, \mu_i^{2I})\, Q_i^I,$$

where $0 < \mu_i^{1I}, \mu_i^{2I} < c$ are constants and Q_i^I are orthogonal 2×2 matrices, $i = 0, \ldots, m$, $I \in \mathcal{I}$. We define

$$\varphi_0^I := \max_{i=0,\ldots,m} \arccos \frac{\min(\mu_i^{1I}, \mu_i^{2I})}{\max(\mu_i^{1I}, \mu_i^{2I})}, \quad \varphi_0^* := \max_{I \in \mathcal{I}} \varphi_0^I. \tag{4.1}$$

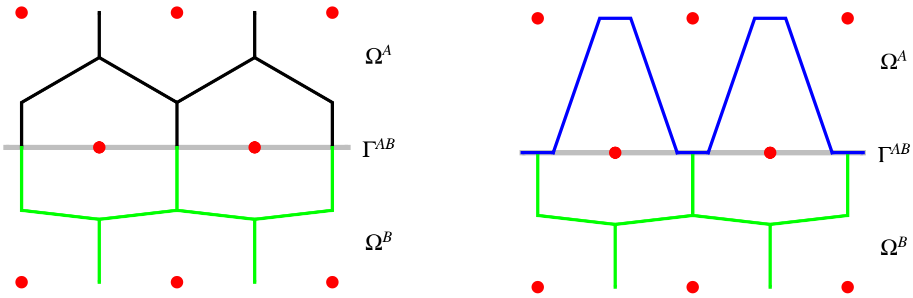

Figure 2: Discretization near a heterostructure interface Γ^{AB}. Left: Compensation of fluxes through the heterostructure interface by two opposite laying Voronoi boxes is guaranteed. Right: Compensation of fluxes by two opposite laying Voronoi boxes only can not be achieved.

We consider a grid $\{x^k : x^k \in \overline{\Omega}, k = 1, \dots, \widetilde{M}\}$ which respects all interfaces Γ^{AB}, $A, B \in \mathcal{I}$, with $|\Gamma^{AB}| > 0$. Especially, the end points of Γ^{AB} are grid points. To apply the methods from Section 3 we want to evaluate fluxes through inner heterostructure interfaces by compensation arguments for the fluxes at the boundary of Voronoi boxes laying opposite to each other with respect to the interface. Figure 2, left shows the desired situation, the compensation can be achieved by the two opposite laying Voronoi boxes only. Figure 2, right depicts an undesired situation which must be excluded. In [10, Lemma 4.2, Remark 4.3] we proved the following criterion for the grid such that compensation by the two opposite laying Voronoi boxes only is possible for all Voronoi boxes defined by the different $\mathbf{S}_i^I$, $i = 0, \dots, m$, $I \in \mathcal{I}$.

For $A, B \in \mathcal{I}$ with $|\Gamma^{AB}| > 0$ we denote by κ^{AB} the quotient of the maximal Euclidian distance of two directly neighboring grid points on the heterostructure interface Γ^{AB} and of the minimal Euclidian distance of inner grid points to the heterostructure interface Γ^{AB}. Then the condition

$$\kappa := \max_{A,\, B \in \mathcal{I},\ |\Gamma^{AB}|>0} \kappa^{AB} \le \sqrt{2 - 2\sin\varphi_0^*} \tag{4.2}$$

where φ_0^* is defined in (4.1) allows to handle general heterostructures and boundary conditions. The severe restriction (4.2) on the placement of vertices on and close to interfaces and boundaries guarantees that the integration procedure described in Section 3 can be applied independently on each Ω^I and the fluxes and potentials fulfill the continuity conditions.
For $Q_i^I = Q^I$ and for straight line interfaces the restriction can be seriously relaxed. But still the largest eigenvalue ratio for each Ω^I defines a forbidden region for interior vertices around the interfaces or boundaries.

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