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Research article

Analysis and finite element approximation of Schrödinger–Poisson system with open Schrödinger boundary conditions

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Abstract: We consider a stationary Schrödinger–Poisson system with open boundary conditions arising in quantum transport modeling. Despite its widespread use in device simulation, the mathematical analysis of such coupled systems remains challenging due to the noncoercivity of the Schrödinger operator and the nonlinear interaction through the electron density and quasi-Fermi level. In this work, we present, to our knowledge, the first comprehensive analysis and finite element framework for the self-consistent system with open boundary conditions. The approach is based on a quasi-Fermi level reparameterization that reveals a monotone structure in the nonlinear Poisson equation and enables a stable decoupling. The resulting formulation combines a Fredholm-based treatment of the Schrödinger equation with a Newton linearization for the Poisson problem, naturally leading to a Gummel-type iteration. We develop finite element discretizations of the subproblems, prove quasi-optimal convergence for the Schrödinger problem and optimal convergence for the Poisson problem, and, using the reparameterization and compactness properties of the electron density, show that, under suitable positivity and boundedness conditions and assuming uniqueness of the fully coupled solution, the finite element iterates converge to that solution. The results provide a consistent and stable theoretical framework for finite element simulations of the Schrödinger–Poisson system and a rigorous basis for numerical methods commonly employed in quantum transport simulations.

Keywords: quantum transport; Schrödinger open boundary conditions; finite element method; Gummel's iteration; error analysis
Mathematics Subject Classification: 65N30, 65N12

1. Introduction

Recent advancements in semiconductor and nanoscale device simulation, particularly in quantum transport regimes, require mathematical models that accurately represent realistic device behavior, motivating rigorous mathematical analysis to further advance the numerical simulation techniques. The

Schrödinger–Poisson system plays a fundamental role in modeling quantum transport in semiconductor devices. Classical studies of stationary Schrödinger–Poisson systems are often formulated as closed systems [1–3], where the Schrödinger equation is equipped with Dirichlet, Neumann, or mixed boundary conditions on bounded domains. These have been extensively studied, establishing existence and, in some cases, uniqueness of solutions under suitable assumptions. However, such boundary conditions suppress carrier transport across the device, whereas semiconductor devices inherently operate through the transport of charge carriers.

To model carrier transport, it is therefore necessary to consider Schrödinger–Poisson systems with open boundary conditions [4–7], which allow particles to enter and leave the domain and thereby enable current flow. Such systems are commonly formulated using scattering-based approaches, including quantum transmitting or transparent boundary condition frameworks. In practice, devices such as nanoscale metal-oxide-semiconductor field-effect transistors (MOSFETs) and related structures are typically described by transport models with open boundary conditions [8–10]. Despite their importance, rigorous analytical results for finite element approximations of stationary Schrödinger–Poisson systems remain limited. Existing works primarily address convergence analysis in the setting of closed quantum systems [11–13].

The transparent boundary condition framework has also been extended beyond the standard effective mass Schrödinger equation to fourth-order and arbitrary order equations incorporating the non-parabolic dispersion effects that captures interference effects absent from the effective mass approximation [14, 15]. Separately, existence and multiplicity of solutions for Schrödinger–Poisson systems in closed settings have been studied extensively using variational methods. They generalize the Schrödinger operator to nonlinear and nonlocal settings, including the p-Laplacian and its fractional extensions, along with critical growth and prescribed mass formulations [16–19]. These works study richer dispersion physics under transparent boundary conditions and existence theory for nonlinear operators under closed boundary conditions, respectively. To the best of our knowledge, there are no comprehensive results on the finite element analysis of stationary Schrödinger–Poisson systems with open boundary conditions.

The objective of this work is to provide such a finite element convergence analysis for the open boundary Schrödinger–Poisson system. We consider a quantum transport model whose finite element discretization follows [6], where the model is rigorously constructed and the existence of solutions is established. Our analysis uses a decoupled Gummel iteration framework [20], solving the coupled system through sequential Schrödinger and Poisson subproblems. We reformulate the coupled system as an iterative scheme and build its well-posedness by proving existence and uniqueness of solutions to each subproblem. We then analyze the finite element approximations, prove quasi-optimal convergence for the Schrödinger problem and optimal convergence for the Poisson problem, and finally show that the Gummel iterates converge to the exact solution of the system.

Self-consistent iterations for open Schrödinger–Poisson systems under nonequilibrium conditions are widely used in numerical simulations [21–23]. In such settings, it is standard to express the carrier density via a quasi-Fermi level, leading to a nonlinear relation involving Fermi–Dirac integrals [23], a formulation favored in Gummel-type iterations for its improved numerical stability and convergence. To analyze the convergence of the iterative scheme at the continuous level, we adopt a quasi-Fermi level reparameterization, obtaining the quasi-Fermi variable by inverting the carrier density relation. This induces a monotone structure in the outer iteration and thereby simplifies the convergence analysis, while the nonlinear Poisson subproblem is solved by Newton's method at each iteration.

The paper is organized as follows. In Section 2, we introduce the model problem consisting of the stationary Schrödinger equation coupled with a nonlinear Poisson equation. In Sections 3 and 4, we establish the existence and uniqueness of weak solutions for the Schrödinger and Poisson subproblems, respectively. Since the Schrödinger equation is not coercive for all energies, its well-posedness is obtained via the Fredholm alternative. In Section 4, we further analyze the nonlinear Poisson equation arising from the quasi-Fermi level reparameterization. Existence and uniqueness are established using monotone operator theory, and the problem is then linearized via Newton's method, whose local convergence at the continuous level is proved. In Section 5, we discretize each subproblem by the finite element method and analyze the well-posedness of the corresponding discrete problems. In particular, for the Schrödinger equation, we use analytical techniques for noncoercive finite element approximations. Finally, Section 6 is devoted to the convergence analysis of the overall self-consistent Schrödinger–Poisson iteration. The analysis relies on compactness arguments for the sequence of iterates together with continuity properties of the electron density. In Section 7, we validate the theory through numerical experiments with a manufactured solution that confirm our convergence results.

2. Model problem

The quantum transport model describes charge carrier motion in nanoscale semiconductor devices where quantum-mechanical effects play a dominant role. The Schrödinger–Poisson system captures the mutual dependence between the electronic structure and the electrostatic field within the device.

2.1. Schrödinger equation

Let $\Omega \subset \mathbb{R}^3$ be the device region occupied by the active material with Lipschitz boundary. The stationary Schrödinger equation in the single-electron effective mass approximation is given by

$$-\frac{\hbar^2}{2}\nabla\cdot\left(\frac{1}{m^*(\mathbf{x})}\nabla\psi(\mathbf{x})\right)+V(\mathbf{x})\,\psi(\mathbf{x})=E\,\psi(\mathbf{x}),\qquad \mathbf{x}\in\Omega, \tag{2.1}$$

where $\hbar$ denotes the reduced Planck constant, $m^*(\mathbf{x})$ is the position-dependent effective mass, and E is the energy eigenvalue associated with the wave function ψ. The potential energy is expressed as $V(\mathbf{x}) = V_c(\mathbf{x}) - q\,U(\mathbf{x})$, where $V_c(\mathbf{x})$ denotes the conduction band minimum energy, q is the magnitude of the elementary charge, and $U(\mathbf{x})$ is the electrostatic potential.

2.2. Poisson equation

The electrostatic potential $U(\mathbf{x})$ appearing in $V(\mathbf{x})$ is governed by the Poisson equation

$$-\nabla\cdot(\epsilon(\mathbf{x})\,\nabla U(\mathbf{x}))=\rho(\mathbf{x}),\qquad \mathbf{x}\in\Omega, \tag{2.2}$$

where $\epsilon(\mathbf{x}) = \epsilon_0\,\epsilon_r(\mathbf{x})$ denotes the position-dependent dielectric permittivity, with ϵ_0 the vacuum permittivity and $\epsilon_r(\mathbf{x})$ the relative permittivity of the material. The charge density $\rho(\mathbf{x}) = q\,(N_D^+(\mathbf{x}) - n(U(\mathbf{x})))$ consists of a donor doping concentration $N_D^+(\mathbf{x})$ and the electron density $n(U(\mathbf{x}))$. Appropriate boundary conditions are imposed to close the Poisson problem:

$$U = U_D \quad \text{on } \Gamma_D, \qquad \boldsymbol{\eta}\cdot(\epsilon\nabla U) = 0 \quad \text{on } \Gamma_N,$$

where Γ_D and Γ_N denote the Dirichlet and Neumann parts of the boundary $\Gamma = \partial\Omega$, respectively, and $\boldsymbol{\eta}$ is the outward unit normal. Here, $U_D(\mathbf{x})$ corresponds to an applied voltage, while the homogeneous Neumann condition on Γ_N enforces charge neutrality along insulated boundaries.

2.3. Coupled system

Equations (2.1) and (2.2) together constitute a nonlinear, self-consistent Schrödinger–Poisson system. The Schrödinger equation determines the quantum-mechanical wave functions and corresponding electron density $n(U)$, whereas the Poisson equation computes the electrostatic potential U generated by that density. Iterating between these two equations yields a self-consistent field solution that describes the steady-state quantum transport behavior within the device.

3. Existence and uniqueness of the weak solution to the stationary Schrödinger equation

We consider a bounded convex polyhedral device domain Ω connected to two semi-infinite leads Ω_1 and Ω_2. Its boundary $\Gamma := \partial\Omega$ is partitioned as $\Gamma = \Gamma_0 \cup \Gamma_1 \cup \Gamma_2$, where Γ_1 and Γ_2 are the disjoint contact interfaces with Ω_1 and Ω_2, respectively, while Γ_0 denotes the remaining portion of the boundary. In correspondence with the boundary notation used in the Poisson problem, Γ_0 coincides with the Dirichlet boundary Γ_D while the contact interfaces Γ_1 and Γ_2 together compose the Neumann boundary Γ_N, in which open boundary conditions are imposed to model charge injection from the leads. The stationary Schrödinger equation (2.1) is formulated with the homogeneous Dirichlet condition on Γ_0 and open (transparent) boundary conditions imposed on $\Gamma_1 \cup \Gamma_2$. Multiplying Eq (2.1) by a test function ϕ and applying Green's identity yields

$$\frac{\hbar^2}{2}\int_{\Omega}\frac{1}{m^*}\nabla\psi\cdot\nabla\overline{\phi}\,d\Omega + \int_{\Omega}(V-E)\psi\overline{\phi}\,d\Omega - \sum_{s=1}^{2}\frac{\hbar^2}{2}\int_{\Gamma_s}\frac{1}{m^*}\left(\boldsymbol{\eta}\cdot\nabla\psi\right)\overline{\phi}\,d\Gamma_s = 0. \tag{3.1}$$

In this variational formulation, the Dirichlet condition on Γ_0 is enforced by choosing ϕ that vanishes on Γ_0, while the open boundary conditions are naturally incorporated through the boundary integral term.

We first analyze the boundary integral in (3.1). For each lead $\Omega_s (s = 1, 2)$, we introduce local coordinates $(\boldsymbol{\xi}_s, \zeta_s)$, where $\boldsymbol{\xi}_s \in \Gamma_s$ is the transverse coordinate and $\zeta_s \in \mathbb{R}^+$ is the longitudinal coordinate along the transport direction. In the leads, the effective mass is assumed to be a constant m_s^*, and the potential depends only on $\boldsymbol{\xi}_s$, so the stationary wave function separates into transverse and longitudinal components. The transverse modes $\varphi_r \in H_0^1(\Gamma_s)$ solve the local Schrödinger eigenvalue problem with eigenvalues E_r and form an orthonormal basis of $L^2(\Gamma_s)$ by spectral theory [24]; the dependence on s is suppressed when the meaning is clear. Based on separation of variables, the wave function is expanded as $\psi_s(\boldsymbol{\xi}, \zeta) = \sum_{r=1}^{\infty}\varphi_r(\boldsymbol{\xi})g_r(\zeta)$, and substituting into Eq (2.1) gives $-\frac{\hbar^2}{2m_s^*}\frac{d^2 g_r}{d\zeta^2} = (E - E_r)\, g_r$ for each mode. For a given total energy E, let $N^s(E)$ be the largest transverse mode index in the s-th lead with $E > E_r$, so that the modes $r \leq N^s(E)$ correspond to propagating states. At threshold energies $E = E_r$, mode r is classified as evanescent, consistent with the strict inequality $E > E_r$ above. Setting $k_r(E) = \hbar^{-1}\sqrt{2m_s^*|E - E_r|}$, the longitudinal solution is $g_r(\zeta) = d_r e^{-ik_r(E)\zeta} + b_r e^{ik_r(E)\zeta}$, where d_r are the prescribed incoming amplitudes, with $d_r = 0$ for $r > N^s(E)$ by the boundedness of the solution to Eq (2.1). Enforcing continuity at the contact surface, the open boundary condition on each interface

Γ_s takes the form

$$\boldsymbol{\eta}\cdot\nabla\psi=\left.\frac{\partial\psi}{\partial\zeta}\right|_{\Gamma_s}=\sum_{r=1}^{N^s(E)} ik_r(E)\left(-2d_r+\langle\psi,\varphi_r\rangle_{\Gamma_s}\right)\varphi_r-\sum_{r=N^s(E)+1}^{\infty} k_r(E)\,\langle\psi,\varphi_r\rangle_{\Gamma_s}\varphi_r$$

with $\langle\psi,\varphi_r\rangle_{\Gamma_s}:=\int_{\Gamma_s}\psi\varphi_r\,d\boldsymbol{\xi}$. We define

$$\mathcal{X}=\left\{\psi\in H^1(\Omega;\mathbb{C}):\psi=0\text{ on }\Gamma_0,\ \sum_{s=1}^{2}\frac{\hbar^2}{2m_s^*}\sum_{r=1}^{\infty}k_r(E)\left|\langle\psi,\varphi_r\rangle_{\Gamma_s}\right|^2<\infty\right\},\tag{3.2}$$

where $H^1(\Omega;\mathbb{C})$ is the Sobolev space of complex-valued functions whose real and imaginary parts belong to $H^1(\Omega)$. The space $\mathcal{X}$ forms a Hilbert space over the complex field $\mathbb{C}$ equipped with the sesquilinear inner product

$$\langle\psi,\phi\rangle_{\mathcal{X},m^*}=\frac{\hbar^2}{2}\int_\Omega\frac{1}{m^*}\nabla\psi\cdot\nabla\overline{\phi}\,d\Omega+\sum_{s=1}^{2}\frac{\hbar^2}{2m_s^*}\sum_{r=1}^{\infty}k_r(E)\,\langle\psi,\varphi_r\rangle_{\Gamma_s}\overline{\langle\phi,\varphi_r\rangle}_{\Gamma_s},$$

and induced norm $\|\psi\|_{\mathcal{X},m^*}=\sqrt{\langle\psi,\psi\rangle_{\mathcal{X},m^*}}$. Assume $\|V\|_{L^\infty(\Omega)}<M$ for a given $M>0$ and that the effective mass is uniformly bounded, i.e., $0<m_-\le m^*(\mathbf{x})\le m_+<\infty$. This gives the norm equivalence $c_{\min}\|\psi\|_{\mathcal{X}}\le\|\psi\|_{\mathcal{X},m^*}\le c_{\max}\|\psi\|_{\mathcal{X}}$, with $c_{\min}=\min(1,1/\sqrt{m_+})$, $c_{\max}=\max(1,1/\sqrt{m_-})$, and

$$\|\psi\|_{\mathcal{X}}^2=\frac{\hbar^2}{2}\int_\Omega|\nabla\psi|^2\,d\Omega+\sum_{s=1}^{2}\frac{\hbar^2}{2m_s^*}\sum_{r=1}^{\infty}k_r(E)\left|\langle\psi,\varphi_r\rangle_{\Gamma_s}\right|^2.$$

We now transform Eq (3.1) into the following weak problem: For a given $E\in\mathbb{R}$ with $E\ge E_{\min}:=\inf_r E_r$, find $\psi\in\mathcal{X}$ such that

$$a(\psi,\phi)=E\,\langle\psi,\phi\rangle+L(\phi)\qquad\text{for all }\phi\in\mathcal{X},\tag{3.3}$$

where $\langle\cdot,\cdot\rangle$ is the $L^2(\Omega)$ inner product. Here $a:=a_1+a_2$, where a_1, a_2, and L are given by

$$\begin{aligned}
a_1(\psi,\phi)&=\frac{\hbar^2}{2}\int_\Omega\frac{1}{m^*}\nabla\psi\cdot\nabla\overline{\phi}\,d\Omega+\sum_{s=1}^{2}\frac{\hbar^2}{2m_s^*}\sum_{r=1}^{\infty}k_r(E)\,\langle\psi,\varphi_r\rangle_{\Gamma_s}\overline{\langle\phi,\varphi_r\rangle}_{\Gamma_s},\\
a_2(\psi,\phi)&=\int_\Omega V\psi\overline{\phi}\,d\Omega-(i+1)\sum_{s=1}^{2}\frac{\hbar^2}{2m_s^*}\sum_{r=1}^{N^s(E)}k_r(E)\,\langle\psi,\varphi_r\rangle_{\Gamma_s}\overline{\langle\phi,\varphi_r\rangle}_{\Gamma_s},\\
L(\phi)&=-\sum_{s=1}^{2}\frac{\hbar^2}{m_s^*}\sum_{r=1}^{N^s(E)}ik_r(E)d_r\overline{\langle\phi,\varphi_r\rangle}_{\Gamma_s}.
\end{aligned}$$

Here we establish the existence and uniqueness for the weak problem (3.3) by reformulating it as a Fredholm equation of the second kind, following [6] with minor modifications. First, we show the form a is bounded and satisfies Gårding's inequality.

Proposition 3.1. *The sesquilinear form $a(\cdot,\cdot):\mathcal{X}\times\mathcal{X}\to\mathbb{C}$ is bounded, that is, $|a(\psi,\phi)|\le c_a\,\|\psi\|_{\mathcal{X}}\,\|\phi\|_{\mathcal{X}}$ for all $\psi,\phi\in\mathcal{X}$ with some positive constant c_a.*

Proof. The boundedness of $a(\cdot,\cdot)$ can be easily obtained by the Cauchy–Schwarz inequality, the uniform boundedness of m^*, and the boundedness of V. □

Proposition 3.2. *There exist constants* $c_1, c_2 > 0$ *such that* $\mathrm{Re}[a(\psi,\psi)] \geq c_1\|\psi\|_{\mathcal{X}}^2 - c_2\|\psi\|_{L^2(\Omega)}^2$, *where* $\mathrm{Re}[a(\cdot,\cdot)]$ *denotes the real part of* $a(\cdot,\cdot)$.

Proof. From the definition of $a(\psi,\psi)$, we have

$$\mathrm{Re}[a(\psi,\psi)] = \frac{\hbar^2}{2}\int_\Omega \frac{1}{m^*}|\nabla\psi|^2\, d\Omega + \int_\Omega V|\psi|^2\, d\Omega + \sum_{s=1}^{2}\frac{\hbar^2}{2m_s^*}\sum_{r=N^s(E)+1}^{\infty} k_r(E)\left|\langle\psi,\varphi_r\rangle_{\Gamma_s}\right|^2.$$

Since $\{\varphi_r\}$ is an orthonormal basis of $L^2(\Gamma_s)$, the constraints (3.2), the trace theorem, and the Poincaré–Friedrichs inequality yield $\sum_{r=1}^{N^s(E)} k_r(E)\left|\langle\psi,\varphi_r\rangle_{\Gamma_s}\right|^2 \leq c\,\|\psi\|_{L^2(\Gamma_s)}^2 \leq c\,\|\nabla\psi\|_{L^2(\Omega)}^2$. Combining these with the bound on V yields the result. □

Having established boundedness and Gårding's inequality, we reformulate the problem (3.3) as an operator equation. Let $J : \mathcal{X} \to \mathcal{X}'$ be the Riesz map and $A : \mathcal{X} \to \mathcal{X}'$ the operator induced by a through $a(\psi,\phi) = \langle A\psi,\phi\rangle_{\mathcal{X}',\mathcal{X}}$, and set $T := J^{-1}A$, so that $a(\psi,\phi) = \langle T\psi,\phi\rangle_{\mathcal{X}}$, where $\mathcal{X}'$ denotes the dual space of $\mathcal{X}$. Let $f \in \mathcal{X}'$ represent L via $\langle f,\phi\rangle_{\mathcal{X}',\mathcal{X}} = L(\phi)$, and let $K : \mathcal{X} \to \mathcal{X}$ be a compact operator associated with the L^2-inner product term. Then the problem (3.3) is equivalent to $T\psi = EK\psi + J^{-1}f$ on $\mathcal{X}$. Since $\mathcal{X} \subset H^1(\Omega)$ is compactly embedded in $L^2(\Omega)$, then K is compact on $\mathcal{X}$. By Proposition 3.2, choosing $\gamma > 0$ large enough makes $a_\gamma(\psi,\phi) := a(\psi,\phi) + \gamma\langle\psi,\phi\rangle$ coercive, so $T_\gamma := J^{-1}A_\gamma$ is bijective by the Lax–Milgram theorem, and the problem (3.3) reduces to

$$(I - \mathcal{K})\psi = p \quad \text{with } \mathcal{K} := (E+\gamma)T_\gamma^{-1}K, \quad p := T_\gamma^{-1}J^{-1}f, \tag{3.4}$$

where $\mathcal{K}$ is compact on $\mathcal{X}$. By the Fredholm alternative [25, Thm. 6.6], Eq (3.4) is uniquely solvable for each p if and only if the homogeneous problem $(I - \mathcal{K})\psi = 0$ has only the trivial solution.

The homogeneous problem reads $a(\psi,\phi) = E\langle\psi,\phi\rangle$ for all $\phi \in \mathcal{X}$. Testing with $\phi = \psi$ eliminates the propagating mode boundary contributions. Hence the homogeneous problem is equivalent to $a_E(\psi,\phi) = E\langle\psi,\phi\rangle$ for all $\phi \in \mathcal{X}$, where a_E is the symmetric, semi-bounded form given by

$$a_E(\psi,\phi) = \frac{\hbar^2}{2}\int_\Omega \frac{1}{m^*}\nabla\psi\cdot\nabla\overline{\phi} + V\psi\overline{\phi}\, d\Omega + \sum_{s=1}^{2}\frac{\hbar^2}{2m_s^*}\sum_{r=N^s(E)+1}^{\infty} k_r(E)\langle\psi,\varphi_r\rangle_{\Gamma_s}\overline{\langle\phi,\varphi_r\rangle_{\Gamma_s}}.$$

We define the unbounded operator A_E on $L^2(\Omega)$ associated with a_E by

$$A_E\psi = -\frac{\hbar^2}{2}\nabla\cdot\left(\frac{1}{m^*}\nabla\psi\right) + V\psi$$

with domain

$$D(A_E) = \left\{\psi \in \mathcal{X} : \left.\frac{\partial\psi}{\partial\zeta}\right|_{\Gamma_s} = -\sum_{r=N^s(E)+1}^{\infty} k_r(E)\langle\psi,\varphi_r\rangle_{\Gamma_s}\varphi_r \text{ and } \nabla\cdot\left(\frac{1}{m^*}\nabla\psi\right) \in L^2(\Omega)\right\}.$$

Then A_E is densely defined, self-adjoint, and semi-bounded on $L^2(\Omega)$. The domain $D(A_E)$, endowed with the graph norm of A_E, is compactly embedded in $L^2(\Omega)$, so A_E has a compact resolvent. By a classical result [26], its spectrum is purely discrete, consisting of real eigenvalues of finite multiplicity with no finite accumulation point. Then, for a given E, the homogeneous problem admits a nontrivial solution if E belongs to the spectrum of A_E, while the inhomogeneous problem has a unique solution if E lies in the resolvent set of A_E. Thus, the weak problem (3.3) is uniquely solvable for all E except those in $\{E_l\}_{l\geq 1}$, the discrete spectrum of A_E.

Since A_E has a purely discrete spectrum, singularities may occur when the given energy E coincides with an eigenvalue of A_E. To avoid this, we add a small absorption term to the energy E. Then the modified weak problem is formulated as

$$a(\psi, \phi) = (E + i\sigma)\langle \psi, \phi\rangle + L(\phi), \qquad \forall \phi \in \mathcal{X}, \tag{3.5}$$

where $0 < \sigma \ll 1$ is a small absorption parameter. For every $E \geq E_{\min}$, the complex shift $z = E + i\sigma$ is in the resolvent set of A_E, which guarantees the unique existence of a solution. For each pair (s', r'), let $\psi^{\sigma}_{s',r'}(\mathbf{x}, E)$ be the unique solution corresponding to the right-hand side $L(\phi)$ with $d_r = \delta_{r,r'}$ on $\Gamma_{s'}$. The electron density is then defined solely by the contribution of the scattering states [6]

$$n(\mathbf{x}) = \sum_{s'=1}^{2} \int_{E_{\min}}^{\infty} f_{s'}(E)\, n_{s'}(\mathbf{x}, E)\, dE, \tag{3.6}$$

where $n_{s'}(\mathbf{x}, E) := \sum_{r'=1}^{N^{s'}} \left|\psi^{\sigma}_{s',r'}(\mathbf{x}, E)\right|^2$, $f_{s'}$ is the Fermi–Dirac occupation function $f_{s'}(E) = 1/(\exp((E - \mu_{s'})\,/\,(k_B T)) + 1)$ with k_B the Boltzmann constant, T the absolute temperature, and $\mu_{s'}$ the electrochemical potential of $\Gamma_{s'}$. This density is then inserted into the Poisson equation to compute the electrostatic potential.

4. Existence and uniqueness of the weak solution to the Poisson equation

In this section, we turn our attention to the nonlinear Poisson equation introduced in Subsection 2.2:

$$-\nabla \cdot \epsilon \nabla U = q\,(N_D^+ - n(U)) \qquad \text{in } \Omega \tag{4.1}$$

with $U = U_D$ on Γ_D and $\boldsymbol{\eta} \cdot (\epsilon \nabla U) = 0$ on Γ_N, which provides electrostatic potential. For Eq (4.1), applying Newton's method before or after deriving the variational (weak) formulation yields the same linear weak form, so we apply Newton's method directly to the weak form of Eq (4.1).

4.1. Variational formulation and Newton's method

We first decompose the solution as $U = U_0 + u$, where U_0 solves $-\nabla \cdot \epsilon \nabla U_0 = q N_D^+$ in Ω with $U_0 = U_D$ on Γ_D and $\boldsymbol{\eta} \cdot (\epsilon \nabla U_0) = 0$ on Γ_N. Once U_0 is obtained, the remaining u satisfies the following nonlinear Poisson equation:

$$-\nabla \cdot (\epsilon \nabla u) = -q\, n\,(U_0 + u) \qquad \text{in } \Omega \tag{4.2}$$

with $u = 0$ on Γ_D and $\boldsymbol{\eta} \cdot (\epsilon \nabla u) = 0$ on Γ_N. We now only focus on Eq (4.2).

For its analysis and linearization, we express the electron density n in terms of the quasi-Fermi level F_n. Specifically, the relation between n and F_n is given by

$$F_n(\mathbf{x}) = V_c(\mathbf{x}) - qU(\mathbf{x}) + k_B T\, \mathcal{F}^{-1}_{1/2}\left(\frac{n\,(U_0(\mathbf{x}) + u(\mathbf{x}))}{N_C}\right), \tag{4.3}$$

where $\mathcal{F}_{1/2}^{-1}$ is the inverse of the complete Fermi–Dirac integral of order $1/2$ and N_C is the effective density of states in the conduction band. Substituting into Eq (4.2) yields the following:

$$-\nabla\cdot(\epsilon(\mathbf{x})\nabla u(\mathbf{x})) = -qN_C\,\mathcal{F}_{1/2}(\alpha(\mathbf{x})+\beta u(\mathbf{x})) =: b(u(\mathbf{x})), \qquad \mathbf{x}\in\Omega, \tag{4.4}$$

where $\alpha(\mathbf{x}) := (k_BT)^{-1}(F_n(\mathbf{x}) - V_c(\mathbf{x}) + qU_0(\mathbf{x}))$ and $\beta := (k_BT)^{-1}q$. We assume $V_c, U_0 \in L^\infty(\Omega)$ and treat α as given. The dependence of α on the electrostatic potential is specified later in Section 6.

The analysis of the nonlinear operator b and the convergence of Newton's method relies on quantitative bounds for $\mathcal{F}_{1/2}$ and its derivatives.

Lemma 4.1. *There exists a constant $c > 0$ such that the following estimates hold for the complete Fermi–Dirac integrals:*

(i) For the order $1/2$ integral, we have

$$\mathcal{F}_{1/2}(\eta) \;\le\; c(1+\eta^{1/2}+\eta^{3/2}) \quad \textit{for all } \eta\ge 0 \tag{4.5}$$

and $\mathcal{F}_{1/2}(\eta)\le c$ for all $\eta\le 0$.

(ii) For the order $-1/2$ integral, we have

$$\mathcal{F}_{-1/2}(\eta) \;\le\; c(1+\eta^{1/2}) \quad \textit{for all } \eta\ge 0 \tag{4.6}$$

and $\mathcal{F}_{-1/2}(\eta)\le c$ for all $\eta\le 0$.

(iii) Let $\mathcal{F}_{-3/2}(\eta) := d^2\mathcal{F}_{1/2}(\eta)/d\eta^2$ via the recursion relation. Then we have

$$\mathcal{F}_{-3/2}(\eta) \;\le\; c \quad \textit{for all } \eta\in\mathbb{R}. \tag{4.7}$$

Proof. We first consider the case $\eta\ge 0$. The definition of the complete Fermi–Dirac integral yields

$$\mathcal{F}_{1/2}(\eta) = \frac{2}{\sqrt{\pi}}\int_0^\infty \frac{\sqrt{t}}{1+e^{t-\eta}}dt = \frac{2}{\sqrt{\pi}}\left(\int_0^\eta \frac{\sqrt{t}}{1+e^{t-\eta}}dt + \int_\eta^\infty \frac{\sqrt{t}}{1+e^{t-\eta}}dt\right),$$

where $\int_0^\eta \sqrt{t}/(1+e^{t-\eta})\,dt \le \int_0^\eta \sqrt{t}\,dt = \frac{2}{3}\eta^{3/2}$ and

$$\begin{aligned}\int_\eta^\infty \frac{\sqrt{t}}{1+e^{t-\eta}}dt &= \int_0^\infty \frac{\sqrt{s+\eta}}{1+e^s}ds \le \int_0^\infty \sqrt{s+\eta}\,e^{-s}ds\\ &= \sqrt{\eta} + \int_0^\infty \frac{e^{-s}}{2\sqrt{s+\eta}}ds \le \sqrt{\eta} + \frac{1}{2}\int_0^\infty s^{-\frac{1}{2}}e^{-s}ds = \sqrt{\eta}+\frac{\sqrt{\pi}}{2}.\end{aligned}$$

Combining the above two inequalities yields inequality (4.5).

For the Fermi–Dirac integral of order $-1/2$, we split the integral as

$$\mathcal{F}_{-1/2}(\eta) = \frac{1}{\sqrt{\pi}}\int_0^\infty \frac{1}{\sqrt{t}\,(1+e^{t-\eta})}dt = \frac{1}{\sqrt{\pi}}\left(\int_0^1 \frac{1}{\sqrt{t}\,(1+e^{t-\eta})}dt + \int_1^\infty \frac{1}{\sqrt{t}\,(1+e^{t-\eta})}dt\right).$$

The first term is uniformly bounded since $\int_0^1 t^{-1/2}(1+e^{t-\eta})^{-1}\,dt \le \int_0^1 t^{-1/2}\,dt = 2$. For the second term, we distinguish two cases, $0\le\eta<1$ and $\eta\ge 1$. If $0\le\eta<1$, then

$$\int_1^\infty \frac{1}{\sqrt{t}\,(1+e^{t-\eta})}dt \le \int_1^\infty e^{-t+\eta}dt \le e\int_1^\infty e^{-t}dt = 1.$$

In the case $\eta \geq 1$, we split at $t = \eta$ and estimate

$$\int_1^\infty \frac{1}{\sqrt{t}\,(1+e^{t-\eta})}dt \leq \int_1^\eta \frac{1}{\sqrt{t}}dt + \int_\eta^\infty e^{-t+\eta}dt = 2\sqrt{\eta} - 1.$$

Again, gathering the above leads us to inequality (4.6).

Using the recursion relation, we have $\mathcal{F}_{-3/2}(\eta) = \pi^{-1/2}\int_0^\infty e^{t-\eta}t^{-1/2}\left(1+e^{t-\eta}\right)^{-2} dt$. We split the integral over $(0,1)$ and $(1,\infty)$. Since $0 < e^{t-\eta}\left(1+e^{t-\eta}\right)^{-2} < 1$, the integral over $(0,1)$ is uniformly bounded. For $(1,\infty)$, we again separate cases. If $0 \leq \eta < 1$, then

$$\int_1^\infty \frac{e^{t-\eta}}{\sqrt{t}\,(1+e^{t-\eta})^2}dt \leq e^\eta \int_1^\infty e^{-t}dt \leq e.$$

If $\eta \geq 1$, then we have

$$\int_1^\infty \frac{e^{t-\eta}}{\sqrt{t}\,(1+e^{t-\eta})^2}dt \leq \int_1^\infty \frac{e^{t-\eta}}{(1+e^{t-\eta})^2}dt = \left[-\frac{1}{1+e^{t-\eta}}\right]_1^\infty = \frac{1}{1+e^{1-\eta}} \leq 1.$$

Hence inequality (4.7) holds for all $\eta \geq 0$.

For $\eta \leq 0$, the bound $e^\eta \leq 1$ applies in all three cases, and the integrands are dominated by integrable functions independent of η. Hence, $\mathcal{F}_{1/2}$, $\mathcal{F}_{-1/2}$, and $\mathcal{F}_{-3/2}$ are all uniformly bounded for $\eta \leq 0$. This completes the proof. □

4.1.1. Variational formulation

We define the solution space by

$$\mathcal{W} = \left\{w \in H^1(\Omega) : w|_{\Gamma_D} = 0\right\}$$

with the dual space $\mathcal{W}'$ and the norm $\|w\|_{\mathcal{W}} := \|w\|_1$, where $\|\cdot\|_1$ is the standard Sobolev $H^1(\Omega)$-norm. The weak problem corresponding to Eq (4.4) is to find $u \in \mathcal{W}$ such that

$$0 = \langle G(u), w\rangle_{\mathcal{W}',\mathcal{W}} := \int_\Omega \epsilon\nabla u \cdot \nabla w \, d\Omega - \int_\Omega b(u)\, w \, d\Omega, \qquad \forall w \in \mathcal{W}, \tag{4.8}$$

where $\langle\cdot,\cdot\rangle_{\mathcal{W}',\mathcal{W}}$ denotes the duality pairing between $\mathcal{W}'$ and $\mathcal{W}$. Accordingly, Eq (4.4) can be equivalently expressed as the operator equation

$$G(u) = 0. \tag{4.9}$$

By the Browder–Minty theorem [27, 28], Eq (4.9) has a unique solution $u \in \mathcal{W}$ provided that G is strictly monotone, coercive, and hemicontinuous. Since the nonlinear term involves $\mathcal{F}_{1/2}$, which is not Lipschitz continuous, hemicontinuity does not follow automatically as in [28] and is verified directly below.

Theorem 4.2. *Assume that α in Eq (4.4) satisfies $\|\alpha\|_{L^2(\Omega)} \leq C$ for some $C > 0$. Then the operator G in Eq (4.9) is monotone, coercive, and hemicontinuous.*

Proof. (*Strong monotonicity*) For any $u, w \in \mathcal{W}$, we have

$$\langle G(u) - G(w), u - w\rangle_{\mathcal{W}',\mathcal{W}} = \int_\Omega \epsilon \left|\nabla (u - w)\right|^2 d\Omega - \int_\Omega (b(u) - b(w))\,(u - w)\,d\Omega.$$

Since $\mathcal{F}_{1/2}$ is monotone increasing, the second integrand is nonpositive, so by the Poincaré–Friedrichs inequality, the above is bounded below by $c\|u - w\|^2_{\mathcal{W}}$ for some $c > 0$.

(*Coercivity*) Taking $w = 0$ in the strong monotonicity bound gives $\langle G(u), u\rangle_{\mathcal{W}',\mathcal{W}} \geq c\|u\|^2_{\mathcal{W}} - \|G(0)\|_{\mathcal{W}'}\|u\|_{\mathcal{W}}$. By Lemma 4.1, the Hölder inequality, and the Sobolev embedding theorem, we obtain

$$\langle G(0), u\rangle_{\mathcal{W}',\mathcal{W}} = qN_C \int_\Omega \mathcal{F}_{1/2}(\alpha)\,u\,d\Omega \leq c\,(1 + \|\alpha\|^{3/2}_{L^2(\Omega)})\,\|u\|_{\mathcal{W}}.$$

Therefore, we get $\langle G(u), u\rangle_{\mathcal{W}',\mathcal{W}} \geq c\left(\|u\|^2_{\mathcal{W}} - \left(1 + \|\alpha\|^{3/2}_{L^2(\Omega)}\right)\|u\|_{\mathcal{W}}\right)$, whose right-hand side tends toward ∞ as $\|u\|_{\mathcal{W}} \to \infty$. Hence the operator G is coercive.

(*Hemicontinuity*) We show that $t \mapsto g(t) := \langle G(u + tv), w\rangle_{\mathcal{W}',\mathcal{W}}$ is continuous on $[0, 1]$ for any $u, v, w \in \mathcal{W}$. Write $g = g_1 - g_2$ with $g_1(t) = \int_\Omega \epsilon\nabla(u + tv)\cdot\nabla w\,d\Omega$ and $g_2(t) = \int_\Omega b(u + tv)\,w\,d\Omega$. Let $\{t_n\} \subset [0, 1]$ converge to some $t \in [0, 1]$. Continuity of g_1 follows from linearity in t. For the nonlinear term g_2, continuity of $\mathcal{F}_{1/2}$ gives $b(u + t_n v) \to b(u + tv)$ pointwise, and by Lemma 4.1, we obtain

$$|b(u + t_n v)\;w| \leq c\left(1 + |\tau_n|^{1/2} + |\tau_n|^{3/2}\right)|w|, \qquad \tau_n := \alpha + \beta u + t_n\beta v,$$

whose right-hand side belongs to $L^1(\Omega)$, since the Hölder inequality together with the Sobolev embedding $H^1(\Omega) \hookrightarrow L^4(\Omega)$ leads to

$$\begin{aligned}\int_\Omega \left(1 + |\tau_n|^{1/2} + |\tau_n|^{3/2}\right)|w|\,d\Omega &\leq c\left(\left(1 + \|\tau_n\|^{\frac{1}{2}}_{L^1(\Omega)}\right)\|w\|_{L^2(\Omega)} + \|\tau_n\|^{\frac{3}{2}}_{L^2(\Omega)}\|w\|_{L^4(\Omega)}\right)\\ &\leq c\left(1 + \|u\|_{L^2(\Omega)} + \|v\|_{L^2(\Omega)}\right)^{\frac{3}{2}}\|w\|_{\mathcal{W}} < \infty.\end{aligned}$$

Consequently, the dominated convergence theorem implies that $g_2(t_n) \to g_2(t)$. Hence g is continuous on $[0, 1]$, and the operator G is hemicontinuous. □

4.1.2. Newton's method

To linearize the problem (4.8), we apply Newton's method, which requires the Fréchet derivative of G. For $u, v \in \mathcal{W}$, let $G'(u)v$ denote this derivative at u in the direction v. By the identity $(\mathcal{F}_p)'(x) = \mathcal{F}_{p-1}(x)$, we have

$$\langle G'(u)v, w\rangle_{\mathcal{W}',\mathcal{W}} = \int_\Omega \epsilon\nabla v\cdot\nabla w\,d\Omega - \int_\Omega b'(u)vw\,d\Omega, \qquad \forall v, w \in \mathcal{W},$$

where $b'(u) = -q\beta N_C\mathcal{F}_{-1/2}(\alpha + \beta u)$. The resulting linearized problem reads as follows: Given an iterate $u_j \in \mathcal{W}$, find the Newton correction $\delta u_j \in \mathcal{W}$ such that

$$\langle G'(u_j)\,\delta u_j, w\rangle_{\mathcal{W}',\mathcal{W}} = -\langle G(u_j), w\rangle_{\mathcal{W}',\mathcal{W}}, \qquad \forall w \in \mathcal{W} \tag{4.10}$$

with update $u_{j+1} = u_j + \delta u_j$ for $j \geq 0$. Equivalently, the Newton step can be expressed in operator form as $G'(u_j)\,\delta u_j = -G(u_j)$ for $j \geq 0$.

Theorem 4.3. *Let $u_j \in \mathcal{W}$ be given and suppose $\|u_j\|_{\mathcal{W}} \leq M$ for some constant $M > 0$. Then the weak problem (4.10) has a unique solution $\delta u_j \in \mathcal{W}$.*

Proof. The bilinear form in (4.10) is continuous by Lemma 4.1 and repeated use of Hölder's inequality. Since $\mathcal{F}_{-1/2}(x) \geq 0$ for all $x \in \mathbb{R}$, there exists $c > 0$ such that

$$\langle G'(u_j)v, v\rangle_{\mathcal{W}',\mathcal{W}} = \int_\Omega \epsilon|\nabla v|^2\, d\Omega + qN_C\beta \int_\Omega \mathcal{F}_{-1/2}(\alpha + \beta u_j)|v|^2\, d\Omega \geq\ c\,\|v\|^2_{\mathcal{W}}$$

for any $v \in \mathcal{W}$. Therefore, the bilinear form is coercive, and the unique solvability of the weak problem (4.10) then follows directly from the Lax–Milgram theorem. □

4.2. Convergence of Newton's method

We now show the local quadratic convergence of Newton's method applied to the operator equation $G(u) = 0$.

Theorem 4.4. *Let $G : \mathcal{W} \to \mathcal{W}'$ be twice Fréchet differentiable in a neighborhood of a solution $u \in \mathcal{W}$ of $G(u) = 0$. Suppose that the Newton iterates $\left\{u_j\right\}$ are well defined and remain in a ball $B_R(u) = \{w \in \mathcal{W} : \|u - w\|_{\mathcal{W}} < R\}$ for some $R > 0$, provided that the initial guess u_0 is chosen sufficiently close to u. Then there exists a constant $c > 0$ such that, with the error $e_j := u - u_j$,*

$$\left\|e_{j+1}\right\|_{\mathcal{W}} \leq c\left\|e_j\right\|^2_{\mathcal{W}} \qquad \textit{for } j = 1, 2, \ldots,$$

which shows that the sequence $\left\{u_j\right\}$ converges quadratically to u in the $\mathcal{W}$-norm.

Proof. Consider Taylor's expansion $0 = G(u) = G(u_j) + G'(u_j)\,e_j + \frac{1}{2}G''(\hat{u}_j)\,[e_j, e_j]$ with $\hat{u}_j = u_j + te_j$ and $t \in (0, 1)$. Using the Newton update and $e_j = u - u_j$,

$$e_{j+1} = u - u_{j+1} = -\frac{1}{2}G'(u_j)^{-1}G''(\hat{u}_j)\,[e_j, e_j].$$

Taking norms and applying the bound for $G'(u_j)^{-1}$, which follows from the coercivity of the bilinear form associated with $G'(u_j)$, gives

$$\left\|e_{j+1}\right\|_{\mathcal{W}} = \frac{1}{2}\left\|G'(u_j)^{-1}G''(\hat{u}_j)[e_j, e_j]\right\|_{\mathcal{W}} \leq c\,\left\|G''(\hat{u}_j)[e_j, e_j]\right\|_{\mathcal{W}'}, \tag{4.11}$$

where the dual norm is $\left\|G''(\hat{u}_j)\,[e_j, e_j]\right\|_{\mathcal{W}'} = \sup_{\|w\|_{\mathcal{W}}=1}\left|\langle G''(\hat{u}_j)\,[e_j, e_j], w\rangle_{\mathcal{W}',\mathcal{W}}\right|$, and the second Fréchet derivative has the form

$$\langle G''(\hat{u}_j)[e_j, e_j], w\rangle_{\mathcal{W}',\mathcal{W}} = q\,N_C\,\beta^2 \int_\Omega \mathcal{F}_{-3/2}(\alpha + \beta\hat{u}_j)\,e_j^2\,w\,d\Omega.$$

Then (4.11), Lemma 4.1, and Hölder's inequality with the Sobolev embedding yield the result. □

5. Finite element discretization

In this section, we discretize the Schrödinger–Poisson model using the finite element method, investigate well-posedness of the discrete subproblems, and analyze the convergence of the finite element approximations.

5.1. Discrete stationary Schrödinger problem

Depending on the parameter regime and the specific formulation, the weak problem for the Schrödinger equation may be coercive or noncoercive. We therefore adopt a unified framework covering both cases and guaranteeing existence and uniqueness of the discrete solution. In the noncoercive case, discrete well-posedness follows from the classical theory for noncoercive finite element approximations developed in [29–31].

Let $\mathcal{T}_h$ be a quasi-uniform, shape-regular tetrahedral triangulation of Ω. We define the finite-dimensional subspace $\mathcal{X}_h \subset \mathcal{X}$ of conforming P_1 finite elements by

$$\mathcal{X}_h := \left\{\phi_h \in C^0(\overline{\Omega}) \cap \mathcal{X} : \phi_h|_T \in P_1(T),\ \forall T \in \mathcal{T}_h\right\},$$

that is, the space of continuous, piecewise linear functions on $\mathcal{T}_h$. Let $\left\{v_j\right\}_{j=1}^{N_h}$ be a real-valued nodal basis of $\mathcal{X}_h$, where N_h denotes the number of degrees of freedom.

We first recall the weak problem (3.5) that seeks $\psi \in \mathcal{X}$ satisfying

$$a_H(\psi, \phi) = L(\phi), \qquad \forall \phi \in \mathcal{X}, \tag{5.1}$$

where $a_H(\psi, \phi) := a(\psi, \phi) - (E + i\sigma)\langle\psi, \phi\rangle$ for a given $E \geq E_{\min}$ and a small absorption parameter $0 < \sigma \ll 1$. Associated with the sesquilinear form a_H, we introduce the adjoint weak problem: Find $w \in \mathcal{X}$ such that

$$a_H^*(w, v) = \langle\psi, v\rangle, \qquad \forall v \in \mathcal{X}, \tag{5.2}$$

where the adjoint form a_H^* is defined by $a_H^*(w, v) := \overline{a_H(v, w)}$. Since $\mathcal{X}$ is a Hilbert space continuously embedded in $L^2(\Omega)$, the right-hand side defines a bounded linear functional on $\mathcal{X}$, hence the adjoint problem is well posed in the same space $\mathcal{X}$. The discrete problem corresponding to the weak problem (5.1) is to find $\psi_h \in \mathcal{X}_h$ for which

$$a_H(\psi_h, \phi_h) = L(\phi_h), \qquad \forall \phi_h \in \mathcal{X}_h. \tag{5.3}$$

We prove the existence and uniqueness of a solution to the discrete problem (5.3) via an error-based stability argument. First, assume that a discrete solution $\psi_h \in \mathcal{X}_h$ exists. Since a_H may not be coercive, uniqueness is not immediate. Expanding $\psi_h = \sum_{j=1}^{N_h} \psi_j v_j$ and $\phi_h = \sum_{l=1}^{N_h} y_l v_l$ with coefficients $\psi_l, y_l \in \mathbb{C}$ and substituting into the problem (5.3) yields

$$\sum_{l=1}^{N_h} \bar{y}_l \left(\sum_{j=1}^{N_h} \psi_j A_{lj} - f_l\right) = 0,$$

where $A_{lj} := a_H(v_j, v_l)$ and $f_l := L(v_l)$. Since the coefficients $\{y_l\}$ are arbitrary, the discrete problem (5.3) is equivalent to the linear system

$$A\boldsymbol{\psi} = \mathbf{f}$$

with $A = (A_{lj})_{l,j=1}^{N_h}$, $\boldsymbol{\psi} = (\psi_j)_{j=1}^{N_h}$, and $\mathbf{f} = (f_l)_{l=1}^{N_h}$. The matrix A is invertible if and only if the homogeneous system $A\boldsymbol{\psi} = \mathbf{0}$ admits only the trivial solution. Therefore, it suffices to show uniqueness through the error estimates under existence assumption, then its existence follows.

We next recall several properties needed for the subsequent result. The continuity of a_H and the validity of Gårding's inequality follow directly from Propositions 3.1 and 3.2. The additional term shifts the continuity constant in Proposition 3.1 by at most $|E| + \sigma$ and modifies the L^2-term in the Gårding inequality of Proposition 3.2 by the same amount. Accordingly, we introduce the associated constants by

$$c_H := c_a + |E| + \sigma, \quad c_1 > 0, \quad \widetilde{c}_2 := c_2 + |E| + \sigma.$$

We further define

$$\theta(\mathcal{X}_h) := \sup_{0\neq z\in L^2(\Omega)} \frac{1}{\|z\|_{L^2(\Omega)}} \inf_{\phi_h\in\mathcal{X}_h} \|w_z - \phi_h\|_{\mathcal{X}}, \tag{5.4}$$

in which $w_z \in \mathcal{X}$ is the solution of the weak problem (5.2) with right-hand side z. The following theorem is based on the argument in [32], adapted appropriately.

Theorem 5.1. *If $\theta(\mathcal{X}_h) \leq \sqrt{c_1}/(c_H\sqrt{2\widetilde{c}_2})$, then the discrete problem (5.3) has a unique solution $\psi_h \in \mathcal{X}_h$ and satisfies quasi-optimal error estimate*

$$\|\psi - \psi_h\|_{\mathcal{X}} \leq 2\, c_H\, c_1^{-1} \inf_{\phi_h\in\mathcal{X}_h} \|\psi - \phi_h\|_{\mathcal{X}}. \tag{5.5}$$

Proof. Let $\psi \in \mathcal{X}$ be the solution of the weak problem (5.1) and let $\psi_h \in \mathcal{X}_h$ solve the discrete problem (5.3). Applying Gårding's inequality to $\psi - \psi_h$, we obtain

$$c_1\, \|\psi - \psi_h\|_{\mathcal{X}}^2 \leq \mathrm{Re}[a_H(\psi - \psi_h, \psi - \psi_h)] + \widetilde{c}_2\, \|\psi - \psi_h\|_{L^2(\Omega)}^2.$$

Using Galerkin orthogonality and the continuity of a_H, we have

$$c_1\, \|\psi - \psi_h\|_{\mathcal{X}}^2 \leq c_H\, \|\psi - \psi_h\|_{\mathcal{X}}\, \|\psi - \phi_h\|_{\mathcal{X}} + \widetilde{c}_2\, \|\psi - \psi_h\|_{L^2(\Omega)}^2 \tag{5.6}$$

for all $\phi_h \in \mathcal{X}_h$. For the duality arguments on $\|\psi - \psi_h\|_{L^2(\Omega)}$, take any $z \in L^2(\Omega)$ and let $w_z \in \mathcal{X}$ solve the adjoint problem (5.2). Setting $\phi = \psi - \psi_h$ in $a_M^*(w_z, \phi) := \overline{a_H(\phi, w_z)}$ yields $|\langle z, \psi - \psi_h\rangle| = |a_H(\psi - \psi_h, w_z)|$. Again, Galerkin orthogonality and continuity of a_H result in

$$|(z, \psi - \psi_h)| \leq c_H\, \|\psi - \psi_h\|_{\mathcal{X}}\, \|w_z - \phi_h\|_{\mathcal{X}}, \qquad \forall \phi_h \in \mathcal{X}_h,$$

which provides

$$\|\psi - \psi_h\|_{L^2(\Omega)} \leq c_H\, \|\psi - \psi_h\|_{\mathcal{X}} \sup_{0\neq z\in L^2(\Omega)} \frac{1}{\|z\|_{L^2(\Omega)}} \inf_{\phi_h\in\mathcal{X}_h} \|w_z - \phi_h\|_{\mathcal{X}}.$$

The definition of $\theta(\mathcal{X}_h)$ in Eq (5.4) leads to $\|\psi - \psi_h\|_{L^2(\Omega)} \leq c_H\theta(\mathcal{X}_h)\, \|\psi - \psi_h\|_{\mathcal{X}}$, and we apply it into inequality (5.6) to obtain

$$c_1\, \|\psi - \psi_h\|_{\mathcal{X}}^2 \leq c_H\, \|\psi - \psi_h\|_{\mathcal{X}}\, \|\psi - \phi_h\|_{\mathcal{X}} + \widetilde{c}_2 (c_H\theta(\mathcal{X}_h))^2\, \|\psi - \psi_h\|_{\mathcal{X}}^2$$

for all $\phi_h \in \mathcal{X}_h$. The given threshold condition for $\theta(\mathcal{X}_h)$ implies $2\widetilde{c}_2(c_H\theta(\mathcal{X}_h))^2 \leq c_1$. Then the last term is absorbed into the left-hand side, which yields inequality (5.5).

Finally, to prove uniqueness of the discrete solution, consider the homogeneous discrete problem. Since the homogeneous continuous problem (3.5) has only the trivial solution $\psi = 0$, the error estimate (5.5) yields

$$\|\psi_h\|_{\mathcal{X}} \leq 2c_H c_1^{-1} \inf_{\phi_h\in\mathcal{X}_h} \|\phi_h\|_{\mathcal{X}} = 0,$$

taking $\phi_h = 0$, thus $\psi_h = 0$. Therefore $A\boldsymbol{\psi} = \mathbf{0}$ has only the trivial solution, then A is invertible, and the discrete problem (5.3) has a unique solution. □

The following shows that $\theta(\mathcal{X}_h)$ decreases proportionally to the mesh size h. Consequently, the threshold condition in Theorem 5.1 holds for sufficiently small h.

Proposition 5.2. *Let Ω be a bounded domain with boundary of class $C^{1,1}$ or a convex polyhedron. Then $\theta(\mathcal{X}_h)$ defined in Eq (5.4) goes to 0 as $h \to 0$.*

Proof. For a given $z \in L^2(\Omega)$, the solution w_z of the adjoint problem (5.2) satisfies $w_z \in H^2(\Omega) \cap \mathcal{X}$ and $\|w_z\|_{H^2(\Omega)} \le c\,\|z\|_{L^2(\Omega)}$ with $c > 0$. Let $J_h w_z \in \mathcal{X}_h$ be the nodal interpolation of w_z. Then the interpolation error estimate and the regularity result give

$$\inf_{\phi_h \in \mathcal{X}_h} \|w_z - \phi_h\|_{\mathcal{X}} \le \|w_z - J_h w_z\|_{\mathcal{X}} \le ch\,|w_z|_{H^2(\Omega)} \le ch\,\|z\|_{L^2(\Omega)}\,. \tag{5.7}$$

So, the arbitrariness of nonzero z in inequality (5.7) with Eq (5.4) leads us to the result. □

From the above, we derive the convergence of finite element approximation.

Proposition 5.3. *The finite element solution ψ_h of the discrete problem (5.3) converges to the exact solution ψ of the problem (5.1) in $\mathcal{X}$ as $h \to 0$.*

Proof. The result follows from Theorem 5.1 and Proposition 5.2. □

5.2. Discrete Poisson problem

Let $\mathcal{T}_h$ be the triangulation of Ω introduced in the previous subsection. We consider the conforming P_1 finite element space

$$\mathcal{W}_h := \left\{ w_h \in C^0(\overline{\Omega}) \cap \mathcal{W} : w_h|_T \in P_1(T) \text{ for all } T \in \mathcal{T}_h \right\}$$

with a real-valued nodal basis $\{\chi_l\}_{l=1}^{N_h}$, where N_h denotes the number of degrees of freedom.

Corresponding to the continuous nonlinear Poisson problem (4.8), the discrete nonlinear problem is to find $u_h \in \mathcal{W}_h$ such that

$$0 = \langle G(u_h), w_h \rangle_{\mathcal{W}',\mathcal{W}}, \qquad \forall w_h \in \mathcal{W}_h. \tag{5.8}$$

Theorem 4.2 shows that G is strongly monotone, that is, there exists a constant $m_G > 0$ such that

$$\langle G(v) - G(z), v - z \rangle_{\mathcal{W}',\mathcal{W}} \ge m_G \|v - z\|^2_{\mathcal{W}}, \qquad \forall v, z \in \mathcal{W}. \tag{5.9}$$

Here the constant m_G depends only on the problem data and the domain.

Proposition 5.4. *The discrete nonlinear Poisson problem* (5.8) *has a unique solution $u_h \in \mathcal{W}_h$.*

Proof. By Theorem 4.2, the operator G is coercive and hemicontinuous on $\mathcal{W}$ and hence also on its finite-dimensional subspace $\mathcal{W}_h$. Therefore, the restriction of G to $\mathcal{W}_h$ has a zero. The uniqueness is easily obtained from the strong monotonicity of G (5.9). □

To compute u_h, we apply Newton's method to (5.8). Given a current Newton iterate $u_{h,j} \in \mathcal{W}_h$, the discrete Newton correction $\delta u_{h,j} \in \mathcal{W}_h$ is defined by

$$\langle G'(u_{h,j})\,\delta u_{h,j}, w_h \rangle_{\mathcal{W}',\mathcal{W}} = -\langle G(u_{h,j}), w_h \rangle_{\mathcal{W}',\mathcal{W}}, \qquad \forall w_h \in \mathcal{W}_h. \tag{5.10}$$

The Newton iterate is then updated according to $u_{h,j+1} = u_{h,j} + \delta u_{h,j}$.

Proposition 5.5. *For every $j \geq 0$, the linearized problem* (5.10) *has a unique solution $\delta u_{h,j} \in \mathcal{W}_h$.*

Proof. The proof is analogous to the proof of Theorem 4.3. The bilinear form associated with the linearized operator is now $(v_h, w_h) \longmapsto \langle G'(u_{h,j})v_h, w_h\rangle_{\mathcal{W}',\mathcal{W}}$. The continuity properties of the nonlinear term imply that this bilinear form is continuous on $\mathcal{W}_h \times \mathcal{W}_h$. Moreover, the ellipticity of the differential part and the monotonicity of $\mathcal{F}_{1/2}$ provide the coercivity of the linearized bilinear form on $\mathcal{W}_h$. Thus the Lax–Milgram theorem then gives the existence and uniqueness of $\delta u_{h,j}$. □

5.2.1. Finite element error and convergence of the discrete Newton iteration

We now separate the finite element discretization error from the error arising from the Newton iteration. Let $u \in \mathcal{W}$ be the solution of the continuous nonlinear problem (4.8), and let $u_h \in \mathcal{W}_h$ be the solution of the discrete nonlinear problem (5.8). The total error of a discrete Newton iterate satisfies

$$\|u - u_{h,j}\|_{\mathcal{W}} \leq \|u - u_h\|_{\mathcal{W}} + \|u_h - u_{h,j}\|_{\mathcal{W}}. \tag{5.11}$$

The first term is the finite element discretization error of the nonlinear Poisson problem, where the second is the error of the discrete Newton iteration. We estimate these terms separately.

For the finite element error estimate, we use the local Lipschitz continuity of G. We assume that there exists a convex bounded neighborhood $\mathcal{B}_R \subset \mathcal{W}$ containing u and u_h and a constant $c > 0$, independent of h, such that

$$\|G(v) - G(z)\|_{\mathcal{W}'} \leq c\,\|v - z\|_{\mathcal{W}}, \qquad \forall v, z \in \mathcal{B}_R. \tag{5.12}$$

This local estimate follows from the continuity properties of the differential part and the local Lipschitz continuity of the Fermi–Dirac term on the bounded range determined by $\mathcal{B}_R$.

Proposition 5.6. *Let $u \in \mathcal{W}$ and $u_h \in \mathcal{W}_h$ be the solutions of* (4.8) *and* (5.8)*, respectively. Suppose that* (5.12) *holds. Then there is a constant $c > 0$ satisfying*

$$\|u - u_h\|_{\mathcal{W}} \leq c \inf_{v_h \in \mathcal{W}_h} \|u - v_h\|_{\mathcal{W}}. \tag{5.13}$$

Proof. For any $v_h \in \mathcal{W}_h$, we write $u - u_h = (u - v_h) + (v_h - u_h)$. Since $v_h - u_h \in \mathcal{W}_h$, the continuous and discrete problems give the nonlinear Galerkin orthogonality $\langle G(u) - G(u_h), v_h - u_h\rangle_{\mathcal{W}',\mathcal{W}} = 0$. Galerkin orthogonality with strong monotonicity established in Theorem 4.2 and (5.12) follow that

$$\|u - u_h\|^2_{\mathcal{W}} \leq c\,\langle G(u) - G(u_h), u - v_h\rangle_{\mathcal{W}',\mathcal{W}} \leq c\,\|G(u) - G(u_h)\|_{\mathcal{W}'}\|u - v_h\|_{\mathcal{W}} \leq c\,\|u - u_h\|_{\mathcal{W}}\|u - v_h\|_{\mathcal{W}},$$

which leads us to (5.13). □

Theorem 5.7. *We consider that the assumptions of Proposition 5.6 hold and suppose that $u \in H^2(\Omega) \cap \mathcal{W}$. Then there exists a constant $c > 0$, independent of h, such that*

$$\|u - u_h\|_{\mathcal{W}} \leq c\,h\,|u|_{H^2(\Omega)}. \tag{5.14}$$

Proof. Let $\Pi_h : H^2(\Omega) \cap \mathcal{W} \longrightarrow \mathcal{W}_h$ be the standard finite element interpolation operator. By taking $v_h = \Pi_h u$ in (5.13) and using interpolation error estimates, the inequality (5.14) is easily obtained. □

We next estimate the second term on the right-hand side of (5.11). We assume that there exists a convex neighborhood $\mathcal{B}_r \subset \mathcal{B}_R$ containing u_h and constants $m_N, L_N > 0$, independent of h, such that

$$\langle G'(v)w, w\rangle_{\mathcal{W}',\mathcal{W}} \geq m_N\|w\|_{\mathcal{W}}^2, \qquad \forall v \in \mathcal{B}_r, \quad \forall w \in \mathcal{W}, \tag{5.15}$$

and

$$\|G'(v) - G'(z)\|_{\mathcal{L}(\mathcal{W},\mathcal{W}')} \leq L_N\|v - z\|_{\mathcal{W}}, \qquad \forall v, z \in \mathcal{B}_r. \tag{5.16}$$

The coercivity in (5.15) follows from the same ellipticity and monotonicity structure used in Theorem 4.2. The local Lipschitz estimate (5.16) follows from the local regularity of the derivative of the Fermi–Dirac term on $\mathcal{B}_r$.

We additionally impose a mesh-uniform condition on the initial Newton approximation: There exist $h_0 > 0$ and $r_N > 0$, independent of h, such that

$$\sup_{0<h\leq h_0} \|u_h - u_{0,h}\|_{\mathcal{W}} \leq r_N \tag{5.17}$$

and that $\mathcal{B} := \{v \in \mathcal{W} : \|v - u_h\|_{\mathcal{W}} \leq r_N\} \subset \mathcal{B}_r$ for $0 < h \leq h_0$. We choose r_N sufficiently small so that

$$q_N := \frac{L_N}{2m_N} r_N < 1. \tag{5.18}$$

Thus all discrete Newton iterations begin in a common convergence neighborhood whose size does not depend on h.

Theorem 5.8. *Suppose that* (5.15)–(5.18) *hold. Then, for every* $0 < h \leq h_0$*, the discrete Newton iterates are well defined, remain in* $\mathcal{B}_r$*, and satisfy*

$$\|u_h - u_{h,j+1}\|_{\mathcal{W}} \leq \frac{L_N}{2m_N}\|u_h - u_{h,j}\|_{\mathcal{W}}^2. \tag{5.19}$$

Moreover, we have

$$u_{h,j} \longrightarrow u_h \quad \text{in } \mathcal{W}$$

quadratically as $j \to \infty$ *and uniformly for* $0 < h \leq h_0$.

Proof. Set $e_{h,j} := u_h - u_{h,j}$. Since u_h satisfies (5.8), we have $\langle G(u_h), w_h\rangle_{\mathcal{W}',\mathcal{W}} = 0$ for all $w_h \in \mathcal{W}_h$. Using (5.10) and $u_{h,j+1} = u_{h,j} + \delta u_{h,j}$ yields

$$\langle G'(u_{h,j})\, e_{h,j+1}, w_h\rangle_{\mathcal{W}',\mathcal{W}} = \Big\langle G'(u_{h,j})\, e_{h,j} - (G(u_h) - G(u_{h,j})), w_h\Big\rangle_{\mathcal{W}',\mathcal{W}}, \ \ \forall w_h \in \mathcal{W}_h. \tag{5.20}$$

Define a path $\phi(t) := G(u_{h,j} + te_{h,j}),\ 0 \leq t \leq 1$. Applying the fundamental theorem of calculus to the continuously Fréchet differentiable operator G along this path gives

$$G(u_h) - G(u_{h,j}) = \phi(1) - \phi(0) = \int_0^1 \phi'(t)\, dt = \int_0^1 G'(u_{h,j} + te_{h,j})\, e_{h,j}\, dt.$$

Therefore, the above leads to $G'(u_{h,j})\, e_{h,j} - (G(u_h) - G(u_{h,j})) = \int_0^1 \Big(G'(u_{h,j}) - G'(u_{h,j} + te_{h,j})\Big)\, e_{h,j}\, dt$. Using (5.16), we obtain

$$\Big\|G'(u_{h,j})e_{h,j} - (G(u_h) - G(u_{h,j}))\Big\|_{\mathcal{W}'} \leq \int_0^1 \Big\|\Big(G'(u_{h,j}) - G'(u_{h,j} + te_{h,j})\Big)\, e_{h,j}\Big\|_{\mathcal{W}'}\, dt$$

$$\leq \int_0^1 \left\| G'(u_{h,j}) - G'(u_{h,j} + te_{h,j}) \right\|_{\mathcal{L}(\mathcal{W},\mathcal{W}')} \|e_{h,j}\|_{\mathcal{W}}\, dt \leq \int_0^1 L_N\, t\, \|e_{h,j}\|_{\mathcal{W}}^2\, dt = \frac{L_N}{2}\|e_{h,j}\|_{\mathcal{W}}^2. \tag{5.21}$$

Taking $w_h = e_{h,j+1}$ in (5.20) and using (5.15) and (5.21), we find

$$m_N\|e_{h,j+1}\|_{\mathcal{W}}^2 \leq \frac{L_N}{2}\|e_{h,j}\|_{\mathcal{W}}^2\|e_{h,j+1}\|_{\mathcal{W}}.$$

Dividing by $\|e_{h,j+1}\|_{\mathcal{W}}$ provides the quadratic convergence of discrete Newton iteration (5.19).

Now we set $\gamma_N := L_N/(2m_N)$. By (5.17), the initial error satisfies $\|e_{0,h}\|_{\mathcal{W}} \leq r_N$. Since $q_N = \gamma_N r_N < 1$ from (5.18), induction yields

$$\|u_h - u_{h,j}\|_{\mathcal{W}} = \|e_{h,j}\|_{\mathcal{W}} \;\leq\; r_N q_N^{2^j-1}, \qquad \forall j \geq 0,$$

and thus $\|e_{h,j}\|_{\mathcal{W}} \leq r_N$. Therefore, the iterates $u_{h,j}$ remain in $\mathcal{B} \subset \mathcal{B}_r$, and the preceding estimates remain valid at every Newton step. Since $q_N < 1$, we have $r_N q_N^{2^j-1} \to 0$ as $j \to \infty$ uniformly for $0 < h \leq h_0$. This proves the result. □

Combining Theorems 5.7 and 5.8 with (5.11), we obtain

$$\|u - u_{h,j}\|_{\mathcal{W}} \leq \|u - u_h\|_{\mathcal{W}} + \|u_h - u_{h,j}\|_{\mathcal{W}} \leq c\, h\, |u|_{H^2(\Omega)} + r_N q_N^{2^j-1}, \tag{5.22}$$

where the constants in both terms on the right-hand side are independent of h. It follows that

$$\|u - u_{h,j}\|_{\mathcal{W}} \longrightarrow 0 \qquad \text{as } j \to \infty,\ h \to 0. \tag{5.23}$$

The estimates established in this subsection provide separate and mesh-uniform control of the finite element discretization error and the inner Newton iteration error for each nonlinear Poisson subproblem. In the next section, these results are incorporated into the outer Gummel iteration to analyze the overall convergence of the fully coupled Schrödinger–Poisson system.

6. Convergence of the Schrödinger–Poisson system

The coupling enters through the right-hand side of the Poisson equation, which depends on the quasi-Fermi level F_n. This quantity is determined by the electron density $n(u)$, which is itself computed from the Schrödinger wave functions associated with the potential u. This mutual dependence constitutes the primary source of nonlinearity in the system, and the resulting nonlinear coupling is handled using a decoupled Gummel iteration.

Let (U^*, ψ^*) denote the solution of the coupled Schrödinger–Poisson system, where $U^* = U_0 + u^*$. Since the reference potential U_0, defined in Section 4, is fixed, the analysis reduces to establishing convergence of the potential sequence toward u^*; convergence of $\{U^l\}$ then follows directly. For convenience, we write $n(u^l)$ for $n(U_0 + u^l)$. To analyze convergence, we recall the iterative procedure. Starting from an initial guess $u^0 \in L^\infty(\Omega)$ and given u^l for $l \geq 0$, we first solve the Schrödinger equation for ψ^{l+1}, then update the potential by solving the Poisson equation for u^{l+1}. The Schrödinger step is stated as follows: For a given u^l, find $\psi^{l+1} \in \mathcal{X}$ such that

$$a_H\left(\psi^{l+1}, \phi\right) = L(\phi), \qquad \forall \phi \in \mathcal{X}, \tag{6.1}$$

where a_H is defined in the weak problem (5.1) with potential energy term $V(u^l) = V_c - qU_0 - qu^l$. The Poisson step reads: For a given ψ^{l+1}, find $u^{l+1} \in \mathcal{W}$ such that

$$\int_\Omega \epsilon \nabla u^{l+1} \cdot \nabla w \, d\Omega = -\int_\Omega qN_C \mathcal{F}_{1/2}\left(\alpha(u^l) + \beta u^{l+1}\right) w \, d\Omega, \qquad \forall w \in \mathcal{W}, \tag{6.2}$$

in which $\alpha(u^l)$ and the quasi-Fermi level $F_n(u^l)$ are evaluated as defined in Section 4.1 with $u = u^l$. The coupled system is thus solved through the iteration

$$u^0 \to \psi^1 \to u^1 \to \psi^2 \to u^2 \to \cdots,$$

which generates a sequence $\{(u^l, \psi^l)\}_{l\geq 1}$.

The well-posedness of each subproblem was established in the previous sections, which ensures that the iteration is well defined. In Section 3, we showed the well-posedness of the Schrödinger problem giving the existence and uniqueness of ψ^{l+1} for a given u^l. The relation in Eq (4.3) in Subsection 4.1 provides the well-posedness of the Poisson problem, which ensures the existence and uniqueness of u^{l+1} for given u^l and quasi-Fermi level $F_n(u^l)$.

Since the $\mathcal{X}$- and $\mathcal{W}$-norms are equivalent to the $H^1(\Omega)$-norm, we write $\|\cdot\|_1$ for the $H^1(\Omega)$-norm in place of $\|\cdot\|_{\mathcal{X}}$ and $\|\cdot\|_{\mathcal{W}}$. To establish the convergence of the finite element iterates to the solution (u^*, ψ^*) of the coupled system, we decompose the errors as

$$\|u^* - u^l_{h,j}\|_1 \leq \|u^* - u^l\|_1 + \|u^l - u^l_{h,j}\|_1 \quad \text{and} \quad \|\psi^* - \psi^l_h\|_1 \leq \|\psi^* - \psi^l\|_1 + \|\psi^l - \psi^l_h\|_1.$$

For each fixed l, the results of Section 5, in particular (5.23), give $\|u^l - u^l_{h,j}\|_1 \to 0$ as $j \to \infty$ and $h \to 0$, while the finite element convergence of the Schrödinger approximation gives $\|\psi^l - \psi^l_h\|_1 \to 0$ as $h \to 0$. It therefore suffices to verify that the outer Gummel iteration errors satisfy

$$\|u^* - u^l\|_1 \to 0, \qquad \|\psi^* - \psi^l\|_1 \to 0 \qquad \text{as } l \to \infty.$$

To proceed, we show that the difference between the wave functions can be controlled by the difference between the electrostatic potentials, under the assumption that $u^*, u^l \in L^\infty(\Omega)$. The analysis relies on the following assumptions.

Assumption 6.1. *The electron density satisfies* $0 < n(\mathbf{x}) \leq \delta$ *for almost everywhere* $\mathbf{x} \in \Omega$.

Assumption 6.2. *The sequence* $\{u^l\}_{l\geq 0} \subset \mathcal{W}$ *is uniformly bounded in* $L^{9/2}(\Omega)$*, that is, there is a constant* $M_u > 0$ *independent of* l *such that* $\|u^l\|_{L^{9/2}(\Omega)} \leq M_u$.

Assumption 6.1 guarantees that the quasi-Fermi level F_n in Eq (4.3) is well defined almost everywhere in Ω. Moreover, by the monotonicity of $\mathcal{F}^{-1}_{1/2}$, the upper bound δ on the electron density provides a uniform upper bound on the inverse Fermi–Dirac term. Assumption 6.2 provides the uniform bound on $\{u^l\}$ required for the regularity in subsequent estimates.

6.1. Continuity estimates

In this subsection, we derive several estimates for the Schrödinger equation that will be used in the convergence analysis.

Proposition 6.3. *Let $u^l \in L^\infty(\Omega)$ and let ψ^{l+1} be the solution of the problem (6.1). Then we have*

$$\left\|\psi^{l+1}\right\|_1^2 \leq c_1(E),$$

where $c_1(E)$ is a positive constant that is independent of l.

Proof. Taking $\phi = \psi^{l+1}$ in (6.1) and separating real and imaginary parts, we first obtain an $L^2(\Omega)$-estimate for ψ^{l+1}. From the imaginary part, using positivity of the propagating modes, we have $\left\|\psi^{l+1}\right\|_{L^2(\Omega)}^2 \leq c(E)$. From the real part, using that $V(u^l) \in L^\infty(\Omega)$, we obtain $\|\nabla\psi^{l+1}\|_{L^2(\Omega)}^2 \leq c(E)\left(\|\psi^{l+1}\|_{L^2(\Omega)}^2 + 1\right)$. Combining the above and applying Poincaré–Friedrichs inequality yields the result. ◻

Building on these bounds, we show that the difference between the wave functions is controlled by the difference in the electrostatic potentials. In particular, convergence of $u^l \to u^*$ in $L^\infty(\Omega)$ implies $\psi^{l+1} \to \psi^*$ in $H^1(\Omega)$, hence $\psi^l \to \psi^*$.

Proposition 6.4. *Let $u^*, u^l \in L^\infty(\Omega)$ and let ψ^* and ψ^{l+1} be the corresponding solutions of the Schrödinger problem. Then there exists $c(E) > 0$ such that*

$$\left\|\psi^* - \psi^{l+1}\right\|_1 \leq c(E)\left\|u^* - u^l\right\|_{L^\infty(\Omega)}.$$

Proof. Let $\delta\psi := \psi^* - \psi^{l+1}$. Subtracting the weak forms for ψ^* and ψ^{l+1} yields

$$a_H(\delta\psi, \phi) = q\int_\Omega \left(u^* - u^l\right)\psi^{l+1}\overline{\phi}\, d\Omega, \qquad \forall\phi \in \mathcal{X}. \tag{6.3}$$

We choose $\phi = \delta\psi$. Then the positivity of the boundary term and Hölder's inequality in the imaginary part of Eq (6.3) give

$$\sigma\|\delta\psi\|_{L^2(\Omega)}^2 \leq q\left\|u^* - u^l\right\|_{L^\infty(\Omega)}\left\|\psi^{l+1}\right\|_{L^2(\Omega)}\|\delta\psi\|_{L^2(\Omega)}$$

that results in the L^2-bound $\sigma\|\delta\psi\|_{L^2(\Omega)} \leq q\left\|u^* - u^l\right\|_{L^\infty(\Omega)}\left\|\psi^{l+1}\right\|_{L^2(\Omega)}$. The real part of Eq (6.3) leads us to

$$\frac{\hbar^2}{2}\int_\Omega \frac{1}{m^*}|\nabla\delta\psi|^2\, d\Omega + \int_\Omega (V(u^*) - E)|\delta\psi|^2\, d\Omega \leq q\int_\Omega \left|u^* - u^l\right|\left|\psi^{l+1}\right||\delta\psi|\, d\Omega.$$

Using the boundedness of $V(u^*)$, it follows that

$$\|\nabla\delta\psi\|_{L^2(\Omega)}^2 \leq c(E)\|\delta\psi\|_{L^2(\Omega)}^2 + c\left\|u^* - u^l\right\|_{L^\infty(\Omega)}\left\|\psi^{l+1}\right\|_{L^2(\Omega)}\|\delta\psi\|_{L^2(\Omega)}.$$

We combine this estimate with the L^2-bound above and use the uniform bound on ψ^{l+1} from Proposition 6.3 to finally obtain $\|\delta\psi\|_1 \leq c(E)\left\|u^* - u^l\right\|_{L^\infty(\Omega)}$. ◻

6.2. Convergence of the Gummel iteration

Now, we show the convergence of $\{u^l\}$ to the solution of the Schrödinger–Poisson system, first establishing a uniform $W^{2,3}(\Omega)$ bound on the iterates and then using the estimates of Subsection 6.1. Here, $\{u^l\}$ denotes the sequence generated by the Gummel iteration in the problems (6.1) and (6.2).

Proposition 6.5. *Under Assumptions 6.1–6.2, the Poisson right-hand side belongs to $L^3(\Omega)$ uniformly in l, and there exists $c > 0$ independent of l such that $\left\|u^{l+1}\right\|_{W^{2,3}(\Omega)} \leq c$.*

Proof. We set $\eta^l := \alpha(u^l) + \beta u^{l+1}$. Using the definition of $\alpha(u^l)$, we obtain

$$\eta^l = (k_B T)^{-1}\left(F_n(u^l) + qU_0 - V_c\right) + \beta u^{l+1} = \mathcal{F}_{1/2}^{-1}\left(n(u^l)/N_C\right) + \beta(u^{l+1} - u^l).$$

From Assumption 6.1 and monotonicity of $\mathcal{F}_{1/2}^{-1}$, we have $\mathcal{F}_{1/2}^{-1}\left(n(u^l)/N_C\right) \leq \mathcal{F}_{1/2}^{-1}(\delta/N_C) =: c_\delta$. Then the argument η^l is bounded as $\eta^l \leq c_\delta + |\beta|\left(\left|u^{l+1}\right| + \left|u^l\right|\right) =: g^l$. Since $\mathcal{F}_{1/2}$ is increasing, we have $0 < \mathcal{F}_{1/2}(\eta^l) < \mathcal{F}_{1/2}(g^l)$. From Lemma 4.1, the estimate $\|\mathcal{F}_{1/2}(\eta^l)\|_{L^3(\Omega)}^3 \leq c\int_\Omega\left(1 + |\eta^l|^{9/2}\right) d\Omega$ holds. Combining the above argument bound, we get

$$\|\mathcal{F}_{1/2}(\eta^l)\|_{L^3(\Omega)}^3 \leq \|\mathcal{F}_{1/2}(g^l)\|_{L^3(\Omega)}^3 \leq c\int_\Omega\left(1 + |g^l|^{9/2}\right) d\Omega.$$

Moreover, by the uniform $L^{9/2}(\Omega)$ bound in Assumption 6.2,

$$\left\|g^l\right\|_{L^{9/2}(\Omega)} \leq c\left(1 + \left\|u^{l+1}\right\|_{L^{9/2}(\Omega)} + \left\|u^l\right\|_{L^{9/2}(\Omega)}\right) \leq c.$$

Thus, the above implies $\|\mathcal{F}_{1/2}\left(\alpha(u^l) + \beta u^{l+1}\right)\|_{L^3(\Omega)} \leq c$. Therefore, the right-hand side of the Poisson equation belongs to $L^3(\Omega)$, and the elliptic regularity yields $u^{l+1} \in W^{2,3}(\Omega)$. The uniform boundedness of the right-hand side in $L^3(\Omega)$ and Assumption 6.2 implies that u^{l+1} is uniformly bounded in $W^{2,3}(\Omega)$. □

Following the uniform bound for u^{l+1}, we now derive a continuity estimate for the electron density with respect to the electrostatic potential.

Proposition 6.6. *Let $u, v \in L^\infty(\Omega)$ be electrostatic potentials associated with the Schrödinger–Poisson system. Then the following holds:*

$$\|n(u) - n(v)\|_{L^2(\Omega)} \leq c\,\|u - v\|_{L^\infty(\Omega)}.$$

Proof. From the definition of the electron density, we have

$$|n(u) - n(v)| \leq \sum_{s'=1}^{2}\int_{E_{\min}}^{\infty} f_{s'}(E)\,|n_{s'}(u) - n_{s'}(v)|\; dE,$$

where $\psi(u)$ and $\psi(v)$ are wave functions for u and v. By the definition of $n_{s'}$ in Eq (3.6),

$$|n_{s'}(u) - n_{s'}(v)| \leq \sum_{r'=1}^{N^{s'}}\left(|\psi(u)| + |\psi(v)|\right)|\psi(u) - \psi(v)|\,.$$

Applying Cauchy–Schwarz's inequality in E and Ω, together with Sobolev embedding $H^1(\Omega) \hookrightarrow L^4(\Omega)$, we obtain $\|n(u) - n(v)\|_{L^2(\Omega)}^2 \leq c\left(\|\psi(u)\|_1^2 + \|\psi(v)\|_1^2\right)\|\psi(u) - \psi(v)\|_1^2$. Using the uniform $H^1(\Omega)$-bounds for ψ (Proposition 6.3) and the stability estimate for the Schrödinger equation (Proposition 6.4), we obtain the stated estimate for n, which completes the proof. □

Using the above, we are now ready to prove the convergence of the sequence $\{u^l\}$.

Theorem 6.7. *Let Assumptions 6.1 and 6.2 hold. Suppose that the Schrödinger–Poisson system admits a unique solution u^*. Then the sequence $\{u^l\}$ generated by problems* (6.1)–(6.2) *converges to u^* in $L^\infty(\Omega)$.*

Proof. By the previous result, $\{u^l\}$ is uniformly bounded in $W^{2,3}(\Omega)$. Since $\Omega \subset \mathbb{R}^3$ is bounded, the compact embedding $W^{2,3}(\Omega) \hookrightarrow L^\infty(\Omega)$ gives a subsequence $\{u^{l_j}\}$ with $u^{l_j} \to u$ in $L^\infty(\Omega)$. Associated with $\{u^{l_j}\}$, the sequence $\{u^{l_j+1}\}$ satisfies

$$\int_\Omega \epsilon \nabla u^{l_j+1} \cdot \nabla w \, d\Omega = -qN_C \int_\Omega \mathcal{F}_{1/2}(\alpha(u^{l_j}) + \beta u^{l_j+1}) w \, d\Omega.$$

We show that the weak form for u^{l_j+1} converges to the following limit equation:

$$\int_\Omega \epsilon \nabla u \cdot \nabla w \, d\Omega = -qN_C \int_\Omega \mathcal{F}_{1/2}(\alpha(u) + \beta u) w \, d\Omega.$$

By subtracting them, we obtain

$$\int_\Omega \epsilon \nabla(u - u^{l_j+1}) \cdot \nabla w = -qN_C \int_\Omega \Big(\mathcal{F}_{1/2}(\alpha(u) + \beta u) - \mathcal{F}_{1/2}(\alpha(u^{l_j}) + \beta u^{l_j+1}) \Big) w. \tag{6.4}$$

Choosing $w = u - u^{l_j+1}$, by coercivity and Poincaré–Friedrichs inequality, we obtain

$$\int_\Omega \epsilon \left| \nabla(u - u^{l_j+1}) \right|^2 \, d\Omega \geq c \left\| u - u^{l_j+1} \right\|_1^2.$$

Then we split the right-hand side of the equation in (6.4) as $I_1 + I_2$, where

$$\begin{aligned} I_1 &= \int_\Omega \left(\mathcal{F}_{1/2}(\alpha(u) + \beta u) - \mathcal{F}_{1/2}(\alpha(u) + \beta u^{l_j+1}) \right) \left(u - u^{l_j+1} \right) \, d\Omega, \\ I_2 &= \int_\Omega \left(\mathcal{F}_{1/2}(\alpha(u) + \beta u^{l_j+1}) - \mathcal{F}_{1/2}(\alpha(u^{l_j}) + \beta u^{l_j+1}) \right) \left(u - u^{l_j+1} \right) \, d\Omega. \end{aligned}$$

By the monotonicity of $\mathcal{F}_{1/2}$ and the sign of $-qN_C$, the term I_1 is nonpositive and is dropped. For I_2, the uniform $L^\infty(\Omega)$ bound obtained from Proposition 6.5 for u, u^{l_j}, and u^{l_j+1} and the upper bound on the electron density in Assumption 6.1 allow the mean value theorem to be applied uniformly, which gives

$$\left| \mathcal{F}_{1/2}(\alpha(u) + \beta u^{l_j+1}) - \mathcal{F}_{1/2}(\alpha(u^{l_j}) + \beta u^{l_j+1}) \right| \leq c \left(\left| u - u^{l_j} \right| + \left| n(u) - n(u^{l_j}) \right| \right).$$

Consequently, by coercivity, we obtain

$$\left\| u - u^{l_j+1} \right\|_1 \leq c \left(\left\| u - u^{l_j} \right\|_{L^2(\Omega)} + \left\| n(u) - n(u^{l_j}) \right\|_{L^2(\Omega)} \right).$$

The continuity estimate for electron density in Proposition 6.6 yields

$$\left\| u - u^{l_j+1} \right\|_1 \leq c \, \left\| u - u^{l_j} \right\|_{L^\infty(\Omega)}.$$

The convergence $u^{l_j} \to u$ in $L^\infty(\Omega)$ implies $u^{l_j+1} \to u$ in $H^1(\Omega)$. Since $\mathcal{F}_{1/2}$ is continuous, passing to the limit in the weak form shows that u satisfies the Schrödinger–Poisson system, hence (u, ψ) is a solution with $u \in W^{2,3}(\Omega) \cap \mathcal{W}$ and $\psi \in \mathcal{X}$. By the uniqueness assumption, $u = u^*$. Since the limit u^* is unique, the standard subsequence argument implies that the full sequence u^l converges to u^* in $L^\infty(\Omega)$. □

Theorem 6.8. *Under the assumptions of Theorem 6.7, let $u^l_{h,j}$ denote the j-th discrete Newton iterate corresponding to the l-th Gummel iteration and let ψ^l_h denote the finite element approximation of ψ^l. Then we have*

$$\left\|u^* - u^l_{h,j}\right\|_1 \to 0, \qquad \left\|\psi^* - \psi^l_h\right\|_1 \to 0 \qquad \text{as } l \to \infty,\ j \to \infty,\ h \to 0.$$

Here l, j, and h correspond to the outer Gummel iteration, the inner discrete Newton iteration, and the finite-element mesh parameter, respectively.

Proof. By Theorem 6.7 and Proposition 6.4, respectively, $u^l \to u^*$ and $\psi^l \to \psi^*$ in $H^1(\Omega)$. Moreover, (5.23) shows that the combined finite element discretization and discrete Newton iteration error satisfies $\|u^l - u^l_{h,j}\|_1 \to 0$ as $j \to \infty,\ h \to 0$, while Proposition 5.3 gives the discretization error $\|\psi^l - \psi^l_h\|_1$, which vanishes as $h \to 0$. Combining these estimates with the error decomposition from the beginning of this section completes the proof. □

7. Numerical results

In this section, we present numerical experiments to validate the theoretical results established in the preceding sections. We examine the convergence of the outer Gummel iteration and the finite element discretization proved in Theorem 6.8, as well as the convergence rates derived in Proposition 5.3 and Theorem 5.7. To perform that, we employ the method of manufactured solutions for the following normalized Schrödinger–Poisson system:

$$\begin{cases} -\nabla^2\psi + V(U)\,\psi - E\,\psi = f & \text{in } \Omega, \\ -\nabla^2 U = -n(U) + g & \text{in } \Omega, \end{cases} \tag{7.1}$$

where the physical constants are normalized by $\frac{\hbar^2}{2m^*} = \epsilon = q = 1$ and $V(U) = -U$. We take $\Omega = (0,1)^3$ and partition its boundary into $\Gamma_1 = \{x = 0\}$, $\Gamma_2 = \{x = 1\}$, and $\Gamma_0 = \partial\Omega \setminus (\Gamma_1 \cup \Gamma_2)$. The Schrödinger equation is equipped with the homogeneous Dirichlet boundary condition on Γ_0 and open boundary conditions on $\Gamma_1 \cup \Gamma_2$ such as

$$\partial_x\psi + ik\psi = \gamma_{\text{in}} \text{ on } \Gamma_1, \quad \partial_x\psi - ik\psi = 0 \text{ on } \Gamma_2.$$

The boundary condition for the Poisson equation is given by $U = 0$ on Γ_0 and $\boldsymbol{\eta} \cdot U = 0$ on $\Gamma_1 \cup \Gamma_2$.

For numerical verification, we consider a single propagating mode with wavenumber $k > 0$. The manufactured exact solution is given by $(U^*, \psi^*) = \big(\cos(2\pi x)\,\sin(\pi y)\,\sin(\pi z),\ e^{ikx}\sin(\pi y)\,\sin(\pi z)\big)$. The corresponding incoming boundary forcing term on Γ_1 is defined by $\gamma_{\text{in}} := 2ik\sin(\pi y)\,\sin(\pi z)$. Let E_1 denote the numerically computed smallest eigenvalue of the associated two-dimensional eigenvalue problem defined in Section 3 with $V(0,y,z) = V(1,y,z) = -\sin(\pi y)\sin(\pi z)$. The total energy is fixed as $E = 25$, which means only one propagating mode is considered, and the wavenumber is defined by $k = \sqrt{E - E_1}$. On Γ_1, the nonhomogeneous boundary forcing γ_{in} represents the prescribed incoming wave, while the homogeneous condition on Γ_2 represents the outgoing wave. The source terms f and g are chosen such that (U^*, ψ^*) is the solution of problem (7.1): $f = \big(k^2 + 2\pi^2 - U^* - E\big)\,\psi^*$ and $g = -\nabla^2 U^* + n(U^*)$. Since we consider only a single mode, the electron density is prescribed by $n(U^*) = |\psi^*|^2$. Using the quasi-Fermi level formulation introduced in Section 4, $F_n(U) = -U + \mathcal{F}^{-1}_{1/2}(n(U))$, the electron density is rewritten as $n(U) = \mathcal{F}_{1/2}(F_n + U)$. Therefore, the corresponding Gummel iteration is given by

$$\begin{cases} -\nabla^2 \psi^{l+1} + V(U^l)\,\psi^{l+1} - E\,\psi^{l+1} = f, \\ -\nabla^2 U^{l+1} = -\mathcal{F}_{1/2}(F_n(U^l) + U^{l+1}) + g, \quad l = 0, 1, 2, \cdots. \end{cases}$$

In theoretical analysis, Theorem 6.8 establishes that the discrete iterates $\left(U^l_{j,h}, \psi^l_h\right)$ converge to the exact solution (U^*, ψ^*) as $j \to \infty$, $h \to 0$, and $l \to \infty$. For notational simplicity, we denote U^l_h by the discrete solution obtained after convergence of the inner Newton iteration for the l-th Gummel iteration. Accordingly, this manufactured example is used to verify the numerical convergence based on theoretical analysis. Since only one propagating mode is considered, this example does not account for the contributions of multiple propagating and evanescent modes or realistic device configurations.

The computational domain is discretized using uniform tetrahedral elements with mesh size h, and the standard nodal basis functions are employed. As discussed in Section 3, the absorption parameter σ shifts the energy from E to $E + i\sigma$, thereby ensuring unique solvability when E belongs to the discrete spectrum of A_E. In the present experiment, $E = 25$ is outside this spectrum, so the shift is unnecessary, and all reported results are computed with $\sigma = 0$. We also repeated the computation with several small positive values of σ. The relative H^1-errors remained unchanged to the reported precision, while the solutions differed only negligibly from that obtained with $\sigma = 0$, which confirms that the numerical results are insensitive to sufficiently small values of σ. The half-order Fermi–Dirac integrals used in the evaluation of $n(U)$ are computed using the method of Mohankumar [33]. The outer Gummel iteration is initialized with $U^0_h = 0$. At each Gummel iteration l, the nonlinear Poisson equation is solved by Newton's method with the stopping criterion $\|U_{h,j+1} - U_{h,j}\|_{l^\infty} / \|U_{h,j+1}\|_{l^\infty} < 10^{-10}$ for $j = 0, 1, 2, \cdots$ and a maximum of 50 iterations. After convergence of the inner Newton iteration, the resulting discrete solution is denoted by U^l_h. The outer Gummel iteration is stopped when $\|U^{l+1}_h - U^l_h\|_{l^\infty} / \|U^{l+1}_h\|_{l^\infty} < 10^{-8}$ for $l = 0, 1, 2, \cdots$. For a fixed mesh size $h = 1/64$, the convergence of the outer Gummel iteration is shown in Figure 1(a). Figure 1(b) and Table 1 present the combined iteration and discretization errors, with the relative errors computed after the outer Gummel iteration has converged on each mesh. Figure 1(b) displays the finite element convergence of the manufactured potential and wave function in the H^1-norm, while Table 1 reports the corresponding relative H^1-errors and observed convergence rates for U^l_h and ψ^l_h as the mesh size decreases from $h = 1/4$ to $h = 1/64$. Both ψ^l_h and U^l_h exhibit first-order convergence with respect to the mesh size, in agreement with the theoretical estimates of Proposition 5.3 and Theorem 5.7, respectively. This numerically confirms the convergence analysis of both the Gummel iteration and the finite element discretization.

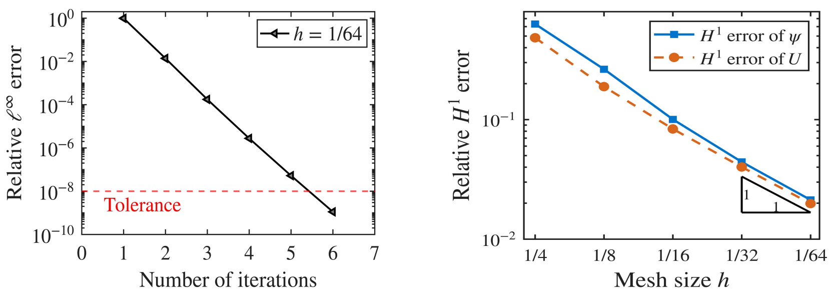

Figure 1. (a) Relative l^∞ difference of electrostatic potential. (b) Relative H^1-error.

Table 1. Relative H^1-errors and their rates: wave function ψ and electrostatic potential U.

mesh size h	$\|\psi^* - \psi_h^l\|_1/\|\psi^*\|_1$	rate	$\|U^* - U_h^l\|_1/\|U^*\|_1$	rate
1/4	6.3023×10^{-1}	–	4.8422×10^{-1}	–
1/8	2.6416×10^{-1}	1.25	1.8874×10^{-1}	1.36
1/16	1.0051×10^{-1}	1.39	8.3546×10^{-2}	1.18
1/32	4.4265×10^{-2}	1.18	4.0130×10^{-2}	1.06
1/64	2.1291×10^{-2}	1.06	1.9850×10^{-2}	1.02

8. Conclusions

In this work, we presented a rigorous finite element analysis of a stationary Schrödinger–Poisson system with open boundary conditions. Although such models are widely used in practical quantum transport simulations and real-world applications, a complete theoretical justification in the open boundary setting has remained largely unavailable. The present work provides, to the best of our knowledge, the first comprehensive analysis to fill this gap. We established the existence and uniqueness of weak solutions for both subproblems, the Schrödinger problem via the Fredholm alternative with an absorption perturbation, and the nonlinear Poisson problem through the quasi-Fermi level formulation with a Newton linearization. We then proved the well-posedness of the finite element discretizations, including the noncoercive Schrödinger case, with quasi-optimal convergence for the Schrödinger problem and optimal convergence for the Poisson problem.

For the fully coupled system under a decoupled Gummel iteration, we decomposed the total error into contributions from the outer Gummel iteration, the inner Newton iteration, and the finite element discretization. Using compactness arguments together with continuity properties of the electron density, we showed that, under suitable positivity and uniform boundedness conditions and assuming uniqueness of the fully coupled solution, the finite element iterates converge to that solution. The analysis is based on a quasi-Fermi level reparameterization that induces a monotone structure in the nonlinear Poisson equation and enables a unified treatment of existence, discretization, and convergence. These results provide a rigorous finite element foundation for open boundary Schrödinger–Poisson simulations extensively used in quantum transport modeling.

Author contributions

Uranchimeg Dorligjav: Formal analysis, investigation, methodology, software, visualization, writing – original draft; Minji Seo: Software, visualization; Eunjung Lee: Conceptualization, formal analysis, investigation, methodology, writing – review & editing. All authors have read and approved the final version of the manuscript for publication.

Use of Generative-AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare no conflicts of interest in this paper.

References

1. F. Nier, Schrödinger–Poisson systems in dimension $d \leq 3$: The whole-space case, *Proc. Roy. Soc. Edinburgh Sect. A,* **123** (1993), 1179–1201. https://doi.org/10.1017/s0308210500029814
2. H. C. Kaiser, J. Rehberg, On stationary Schrödinger–Poisson equations modelling an electron gas with reduced dimension, *Math. Methods Appl. Sci.,* **20** (1997), 1283–1312. https://doi.org/10.1002/(sici)1099-1476(199710)20:15¡1283::aid-mma914¿3.0.co;2-p
3. H. C. Kaiser, J. Rehberg, About a stationary Schrödinger–Poisson system with Kohn–Sham potential in a bounded two- or three-dimensional domain, *Nonlinear Anal.-Theor.,* **41** (2000), 33–72. https://doi.org/10.1016/s0362-546x(98)00261-2
4. W. R. Frensley, Boundary conditions for open quantum systems driven far from equilibrium, *Rev. Mod. Phys.,* **62** (1990), 745–791. https://doi.org/10.1103/revmodphys.62.745
5. C. S. Lent, D. J. Kirkner, The quantum transmitting boundary method, *J. Appl. Phys.,* **67** (1990), 6353–6359. https://doi.org/10.1063/1.345156
6. N. B. Abdallah, On a multidimensional Schrödinger–Poisson scattering model for semiconductors, *J. Math. Phys.,* **41** (2000), 4241–4261. https://doi.org/10.1063/1.533397
7. M. Baro, H. C. Kaiser, H. Neidhardt, J. Rehberg, A quantum transmitting Schrödinger–Poisson system, *Rev. Math. Phys.,* **16** (2004), 281–330. https://doi.org/10.1142/s0129055x04001996
8. O. Kurniawan, P. Bai, E. Li, Ballistic calculation of nonequilibrium Green's function in nanoscale devices using finite element method, *J. Phys. D: Appl. Phys.,* **42** (2009), 105109. https://doi.org/10.1088/0022-3727/42/10/105109
9. E. Lee, U. Dorligjav, R. James, B. Kim, H. U. Cho, S. Baek, A new approach for efficient nonequilibrium quantum transport computation in electroluminescent quantum dots, *Commun. Nonlinear Sci. Numer. Simul.,* **143** (2025), 108638. https://doi.org/10.1016/j.cnsns.2025.108638
10. U. Dorligjav, M. Seo, E. Lee, Theoretical analysis and high-performance implementation of low-rank approximations in NEGF-based quantum transport, *Commun. Nonlinear Sci. Numer. Simul.,* **152** (2026), 109265. https://doi.org/10.1016/j.cnsns.2025.109265
11. L. Zhang, L. Cao, J. Luo, Multiscale analysis and computation for a stationary Schrödinger–Poisson system in heterogeneous nanostructures, *Multiscale Model. Simul.,* **12** (2014), 1561–1591. https://doi.org/10.1137/13091991x

12. T. Cui, W. Lu, N. Pan, W. Zheng, On finite element approximation of the Schrödinger–Poisson model, *Math. Models Methods Appl. Sci.,* **35** (2025), 1297–1324. https://doi.org/10.1142/s0218202525500186

13. T. Cui, W. Lu, N. Pan, W. Zheng, A two-grid finite element method for the Schrödinger–Poisson system, *IMA J. Numer. Anal.,* **46** (2025), 873–898. https://doi.org/10.1093/imanum/draf014

14. G. E. Aliffi, G. Nastasi, V. Romano, Ballistic electron transport described by a fourth-order Schrödinger equation, *Z. Angew. Math. Phys.,* **76** (2025), 155. https://doi.org/10.1007/s00033-025-02535-5

15. G. E. Aliffi, G. Nastasi, V. Romano, Ballistic electron transport described by a generalized Schrödinger equation, *J. Phys. A: Math. Theor.,* **59** (2026), 135201.

16. K. Liu, X. He, Solutions with prescribed mass for the Sobolev critical Schrödinger–Poisson system with p-Laplacian, *Bull. Math. Sci.,* **15** (2025), 2550006. https://doi.org/10.1142/S1664360725500067

17. S. Liang, P. Pucci, T. V. Nguyen, D. Xiao, Multiplicity and concentration of normalized solutions for double critical Schrödinger–Poisson systems involving the fractional p-Laplacian in $\mathbb{R}^3$, *Nonlinear Anal.,* **269** (2026), 114104. https://doi.org/10.1016/j.na.2026.114104

18. X. Ma, S. Shi, Y. Song, Existence of solutions for a doubly critical Schrödinger–Poisson system on the first Heisenberg group, *Opuscula Math.,* **46** (2026), 347–366. https://doi.org/10.7494/OpMath.202605211

19. X. He, S. Liang, P. Pucci, On the double critical p-fractional Schrödinger–Poisson system with electromagnetic fields in $\mathbb{R}^3$, *Adv. Nonlinear Stud.,* **26** (2026), 212–238. https://doi.org/10.1515/ans-2023-0207

20. H. K. Gummel, A self-consistent iterative scheme for one-dimensional steady state transistor calculations, *IEEE Trans. Electron Devices,* **11** (1964), 455–465. https://doi.org/10.1109/t-ed.1964.15364

21. O. Pinaud,Transient simulations of a resonant tunneling diode, *J. Appl. Phys.,* **92** (2002), 1987–1994. https://doi.org/10.1063/1.1494127

22. E. Polizzi, N. B. Abdallah, Subband decomposition approach for the simulation of quantum electron transport in nanostructures, *J. Comput. Phys.,* **202** (2005), 150–180. https://doi.org/10.1016/j.jcp.2004.07.003

23. D. Chen, G. W. Wei, Modeling and simulation of electronic structure, material interface and random doping in nano-electronic devices, *J. Comput. Phys.,* **229** (2010), 4431–4460. https://doi.org/10.1016/j.jcp.2010.02.002

24. L. C. Evans, *Partial differential equations*, 2 Eds., American Mathematical Society, 2010. https://doi.org/10.1090/gsm/019

25. H. Brézis, *Functional analysis, Sobolev spaces and partial differential equations*, Springer, 2011. https://doi.org/10.1007/978-0-387-70914-7

26. M. Reed, B. Simon, *Methods of modern mathematical physics: Functional analysis*, Academic Press, 1972. https://doi.org/10.1016/B978-0-12-585001-8.X5001-6

27. E. Zeidler, *Nonlinear functional analysis and its applications: II/B: nonlinear monotone operators*, Springer, 1990. https://doi.org/10.1007/978-1-4612-0981-2
28. P. Heid, T. Wihler, Adaptive iterative linearization Galerkin methods for nonlinear problems, *Math. Comp.,* **89** (2020), 2707–2734. https://doi.org/10.1090/mcom/3545
29. A. H. Schatz, An observation concerning Ritz-Galerkin methods with indefinite bilinear forms, *Math. Comp.,* **28** (1974), 959–962. https://doi.org/10.1090/s0025-5718-1974-0373326-0
30. A. Schatz, J. Wang, Some new error estimates for Ritz–Galerkin methods with minimal regularity assumptions, *Math. Comp.,* **65** (1996), 19–27. https://doi.org/10.1090/s0025-5718-96-00649-7
31. S. A. Sauter, A refined finite element convergence theory for highly indefinite Helmholtz problems, *Computing,* **78** (2006), 101–115. https://doi.org/10.1007/s00607-006-0177-z
32. E. A. Spence, *Overview of variational formulations for linear elliptic PDEs*, in Unified Transform for Boundary Value Problems (eds. A. S. Fokas and B. Pelloni), Society for Industrial and Applied Mathematics, 2014, 93–159. https://doi.org/10.1137/1.9781611973822.ch6
33. N. Mohankumar, Fermi, *MATLAB central file exchange*, 2026, Available from: `https://www.mathworks.com/matlabcentral/fileexchange/13616-fermi`.

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