

ANALYTIC EXPRESSIONS FOR CURRENT-VOLTAGE CHARACTERISTICS FROM THE QUANTUM HYDRODYNAMIC EQUATIONS

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We consider a simplified one-dimensional steady-state quantum hydrodynamic (QHD) model in which the real-valued potential V is given and not self-consistently coupled to the electron density. The Madelung equivalence between the QHD model and the Schrödinger equation, as well as the appropriate choice of the potential V , allow us to treat the corresponding exactly solvable Schrödinger equation instead of solving a third-order nonlinear QHD system. For a given choice of potential, we give the analytical expression for the current-voltage characteristic. The obtained curves show the effect of negative differential resistance (NDR), where the electric current decreases with increasing bias voltage.

Keywords: quantum hydrodynamics, Madelung transform, Schrödinger equation, current-voltage characteristic, Airy differential equation, confluent hypergeometric function.

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1. Introduction

When dealing with complete quantum models, it is worthwhile to examine the steady-state simulation results (current-voltage curves, possible bistabilities). More specifically, we consider the stationary QHD model in which the real-valued potential $V(x)$ is given and not self-consistently coupled to the electron density. It is well known that the QHD model can be obtained from the Schrödinger equation using the Madelung transformation (3). Instead of solving a third order nonlinear QHD system, one can deal with the equivalent Schrödinger equation, which can be solved exactly for a given potential, and give an explicit formula to calculate the corresponding current-voltage characteristic. When developing algorithms or modeling physical systems, analytical solutions often offer important advantages. They provide direct insight into the effects of the various variables and their interactions on the outcome. The study of exactly solvable Schrödinger equations in the QHD context began in [4], where the author derived the analytical expression for the reduced QHD model with $V(x) = 0$, and was continued by [8], where the linear potential was used. In this article, we go a step further and consider the nonlinear potentials: the monomial and the Morse potential. The inclusion of the pressure term introduces a nonlinearity in the Schrödinger-like equation, which means that we cannot obtain an explicit formula for the current-voltage curve. In

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this case, we give an existence result using the theory for monotone nonlinear operators. We also numerically investigate the influence of the pressure term on the current-voltage characteristic.

The work is organized as follows. After the introduction in section 1, section 2 is devoted to the analytical expressions of the current-voltage curves for the unpressurized QHD model with the monomial and the Morse potential, connecting the Schrödinger equation with the Airy differential equation on one side and the confluent hypergeometric equation on the other. Finally, in section 3 we discuss the influence of the pressure term in the QHD model on the JU curves by performing numerical simulations.

The three-dimensional, time-dependent, nonlinear one-particle Schrödinger equation is as follows:

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2}\Delta\psi + [V(x) + f(|\psi|^2)]\psi, \quad (1)$$

where $\psi = \psi(x, t) \in \mathbb{C}$ is the wave-function, $t \geq 0$, $x \in \mathbb{R}^3$, \hbar is the reduced Planck constant and $V(x)$ is assumed to be a real function that represents the potential energy of the system. The density dependent pressure term $p(n)$ is defined by $p'(n) = nf'(n)$, where the function $f : (0, +\infty) \rightarrow \mathbb{R}$ is the enthalpy of the system. In this article we are interested in the isentropic case, where one has

$$p(n) = \eta n^\gamma, \text{ where } 1 < \gamma < 3 \text{ and } f(n) = \eta \frac{\gamma}{\gamma-1} n^{\gamma-1}, \quad (2)$$

with η a (scaled) temperature constant. Assuming that the equation (1) has a solution, Madelung's idea was to write the complex-valued wave function in the polar form

$$\psi(x, t) = R(x, t)e^{\frac{iS(x, t)}{\hbar}}, \quad (3)$$

where $R(x, t)$ represents the amplitude and $S(x, t)$ is the action function. It is assumed that R is nonnegative at every point. The probability density associated with the wave function is denoted by $n(x, t) = |\psi(x, t)|^2 = R(x, t)^2$. By inserting (3) into (1) we obtain a system of two coupled partial differential equations:

$$\partial_t n + \operatorname{div}(n\nabla S) = 0, \quad (4)$$

$$\partial_t S + \frac{|\nabla S|^2}{2} + f(n) - \frac{\hbar^2}{2} \frac{\Delta\sqrt{n}}{\sqrt{n}} + V = 0. \quad (5)$$

We note here that if the pair (S, n) solves the Madelung system (4)-(5), then the complex-valued wavefunction $\psi(x, t)$ given by (3) solves the Schrödinger equation (1). After we denote the velocity field by $\mathbf{v} = \nabla S$, we obtain the quantum hydrodynamic model (QHD), which consists of the continuity equation and the momentum equation with an additional third-order quantum term:

$$\partial_t n + \operatorname{div}(n\mathbf{v}) = 0, \quad (6)$$

$$\partial_t(n\mathbf{v}) + \nabla \cdot (n\mathbf{v} \otimes \mathbf{v}) + n\nabla V - \nabla p(n) - \frac{\hbar^2}{2} n \nabla \left(\frac{\Delta\sqrt{n}}{\sqrt{n}} \right) = 0. \quad (7)$$

By $J = n\mathbf{v}$ we denote the electron current density, which can be expressed in terms of the wave function by the following expression:

$$J = -\frac{i\hbar}{2} [\bar{\psi} \nabla \psi - \psi \nabla \bar{\psi}] = \hbar \text{Im} (\bar{\psi} \nabla \psi). \quad (8)$$

We note that the boundary conditions for the Schrödinger equation, used in this article, given by

$$\psi(0) = 1, \psi(1) = e^{\frac{iU}{\varepsilon}} \quad (9)$$

are motivated by the boundary conditions used for the QHD model. More precisely, we consider the stationary, one-dimensional QHD model. The corresponding scaling is discussed in [4] and it leads to a model of the form

$$J_x = 0, \quad (10)$$

$$\left(\frac{J^2}{n} + p(n) \right)_x + nV_x - \frac{\varepsilon^2}{2} n \left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}} \right)_x = 0, \quad (11)$$

where ε is a scaled Planck constant. Let the device domain be represented by the spatial (scaled) interval $(0, 1)$. The QHD formulation is equivalent to (10)-(11) reads:

$$(nS_x)_x = 0, \quad (12)$$

$$\frac{S_x^2}{2} + f(n) + V(x) - \frac{\varepsilon^2}{2} \frac{(\sqrt{n})_{xx}}{\sqrt{n}} = 0. \quad (13)$$

We impose that

$$V(0) = 0, V(1) = U, \quad (14)$$

where $U \in \mathbb{R}$ is the applied potential. Physically relevant hypotheses for deriving the boundary conditions for n and S

$$n(0) = n(1) = 1, S(0) = 0, S(1) = U, \quad (15)$$

can be found in [5, 8].

2. Analytic JU-curves for QHD models

We are interested in deriving an analytical expression for the current-voltage curve for a given QHD model directly from the corresponding Schrödinger equation. Let us begin with the simple case where the special form of the potential (linear and monomial) in the Schrödinger equation and the absence of the nonlinear enthalpy term given by the function f allow us to rewrite the Schrödinger equation into an Airy differential equation solvable exactly in terms of Airy functions. Next, we move on to other potentials for which the corresponding Schrödinger equation has an explicit solution. In this direction, we take advantage of the fact that certain Schrödinger-like equations can be transformed into the hypergeometric equation by a gauge transformation and by a certain change of variables. The connection between the one-dimensional Schrödinger equation and the hypergeometric equation was first made by Natanzon, [10]. One of the most important references on hypergeometric functions is the classical book [1].

Our general procedure is to solve the corresponding Schrödinger equation with the given potential $V(x)$ satisfying (14) and the boundary conditions (9), then calculate J with the formula (8) and finally develop the JU curve. We start with the stationary QHD problem (10)-(11) where $x \in (0, 1)$ with boundary conditions (15). In [4] the author derives the analytic expression $J(U) = \varepsilon \sin(U/\varepsilon)$ for the reduced QHD model resulting from the system (12)-(13) by assuming $f(n) = 0$ and $V(x) = 0$, using the boundary conditions (15).

2.1. QHD model with the monomial potential

In this section we consider the QHD model (10)-(11) with given linear and monomial electric potential $V(x)$ and without the pressure term, with $x \in (0, 1)$, where a small parameter ε is the scaled Planck constant. This scaling leads to a corresponding stationary equation of Schrödinger type,

$$\frac{\varepsilon^2}{2}\psi_{xx} - V(x)\psi = 0, \quad x \in (0, 1), \quad (16)$$

which can be solved explicitly in terms of Airy functions using the boundary conditions (9). We mention here the following result from [8].

Proposition 2.1. *For the quantum hydrodynamic model (10)-(11) with $p(n) = 0$ and boundary conditions (9), with linear electric potential $V(x) = xU$, the current-voltage characteristic $J = J(U)$ is given by*

$$J(U) = \frac{\varepsilon}{\pi} \frac{\beta(U) \sin(U/\varepsilon)}{Ai(0)Bi(\beta(U)) - Ai(\beta(U))Bi(0)}. \quad (17)$$

where $\beta(U) = (2U/\varepsilon^2)^{1/3}$. Moreover,

$$J(U) \rightarrow 0, \text{ as } U \rightarrow 0 \quad \text{and} \quad J(U) \rightarrow 0, \text{ as } U \rightarrow \infty. \quad (18)$$

The generalization to the monomial potential $V(x) = x^m U$, for $m \in \mathbb{N}$ follows directly. We consider the Schrödinger equation

$$\frac{\varepsilon^2}{2}\psi_{xx} - x^m U \psi = 0, \quad x \in (0, 1), \quad (19)$$

with the same Dirichlet boundary conditions (9).

By substituting $y = \beta x$, $\beta^{2+m} = 2U/\varepsilon^2$ and $\psi(x) = \varphi(\beta x)$, the Schrödinger equation (19) can be rewritten as

$$\varphi''(y) - y^m \varphi(y) = 0, \quad \text{on } (0, \beta) \quad (20)$$

with the boundary conditions $\varphi(0) = 1$, $\varphi(\beta) = e^{\frac{iU}{\varepsilon}}$. The equation (20) is an extension of Airy's differential equation [12]. It has two independent solutions A_m and B_m which are real for real arguments and agree with the Airy functions for $m = 1$.

Proposition 2.2. *For quantum-hydrodynamic model (10)-(11) with $p(n) = 0$ and the boundary conditions (9), with monomial electric potential $V(x) = x^m U$, $m \in \mathbb{N}$, $U > 0$, the*

current-voltage characteristic, $J = J(U)$, is given by

$$J(U) = \frac{2\varepsilon \sin(\pi/(m+2))}{\sqrt{m+2}\pi} \frac{\beta(U) \sin(U/\varepsilon)}{A_m(0)B_m(\beta(U)) - A_m(\beta(U))B_m(0)}. \quad (21)$$

where $\beta(U) = (2U/\varepsilon^2)^{1/(2+m)}$. Moreover,

$$J(U) \rightarrow 0, \text{ as } U \rightarrow 0 \quad \text{and} \quad J(U) \rightarrow 0, \text{ as } U \rightarrow \infty. \quad (22)$$

Proof. The proof of the expression (21) and the limit $U \rightarrow 0$ is based on the expression

$$J = \varepsilon \operatorname{Im}(\overline{\psi(0)}\psi'(0)) = \varepsilon\beta \operatorname{Im}(\overline{\varphi(0)}\varphi'(0)).$$

and properties of the functions A_m and B_m , notably (see [12]), for $p = 1/(m+2)$, one has

$$\begin{aligned} A_m(0) &= \frac{p^{1-p}}{\Gamma(1-p)}, \quad B_m(0) = \frac{p^{1/2-p}}{\Gamma(1-p)}, \\ A'_m(0) &= -\frac{p^p}{\Gamma(p)}, \quad B'_m(0) = \frac{p^{p-1/2}}{\Gamma(p)}. \end{aligned}$$

The limit as $U \rightarrow \infty$ relies on the fact that $A_m(u)$ goes to zero as $u \rightarrow \infty$, and $B_m(u)$ exponentially grows as $u \rightarrow \infty$. That is a consequence of asymptotic formulas (see [12]):

$$\begin{aligned} A_m(u) &= (p/\pi)^{1/2} \sin(p\pi) u^{-m/4} e^{-w} (1 + O(1/w)), \\ B_m(u) &= \pi^{-1/2} u^{-m/4} e^w (1 + O(1/w)), \end{aligned}$$

for $w = 2/(m+2)$, $u^{(m+2)/2}$. This completes the proof. \square

2.2. QHD model with the Morse potential

There are a number of nonlinear potentials from quantum mechanics for which the Schrödinger equation is exactly solvable. We mention here the Morse, Poschll-Teller, Eckart, and Manning-Rosen potentials (see [2] and references therein). More precisely, according to [9], in each of the above cases there is a gauge function $\sigma(z)$ and a change of variable $z = z(x)$ such that the solutions of the corresponding Schrödinger equation $\psi_{xx}(x) - V(x)\psi(x) = 0$, are of the form $\psi(x) = \exp[\sigma(z(x))]\varphi(z(x))$. Here $\varphi(z)$ is either the Gaussian hypergeometric function or the confluent hypergeometric function, recently interesting for researchers both from theoretical and numerical point of view, [6, 3].

In this section we focus on the current-voltage characteristics for the Schrödinger equation with the Morse potential. This potential is globally increasing and has no singularities, which makes it suitable for calculating the JU curve. The solution of the Schrödinger equation with the Morse potential can be written in terms of confluent hypergeometric functions, i.e. Kummer and Tricomi functions (see [7, 11]).

Let us consider the Schrödinger equation (16) where the potential $V(x)$ is given by the Morse potential (see [2, 9])

$$V_\varepsilon(x) = -\frac{\nu}{2}c_\varepsilon^{-x} + \frac{1}{4}c_\varepsilon^{-2x} + \frac{\alpha^2}{4}, \quad c_\varepsilon = e^{\sqrt{2}/\varepsilon}, \quad (23)$$

which is a function of two parameters, ν and α .

Since we consider the potential $V(x)$ to satisfy $V(0) = 0$, we set $\alpha = \sqrt{2\nu - 1}$, which leads to the one-parameter potential

$$V_\varepsilon(x) = \frac{\nu}{2}(1 - c_\varepsilon^{-x}) - \frac{1}{4}(1 - c_\varepsilon^{-2x}). \quad (24)$$

By imposing $V(1) = U$ we get that we can express the parameters ν and α as functions of U :

$$\begin{aligned} \nu &= \frac{2U}{1 - c_\varepsilon^{-1}} + \frac{1}{2}(1 + c_\varepsilon^{-1}) \geq \frac{1}{2}(1 + c_\varepsilon^{-1}), \\ \alpha &= \sqrt{2\nu - 1} > \sqrt{4U + c_\varepsilon^{-1}}. \end{aligned}$$

By simple calculation it can be shown that the solution of (16) with the potential (24) can be written in the form

$$\psi(x) = H_\varepsilon(x)\phi(c_\varepsilon^{-x}), \quad H_\varepsilon(x) = c_\varepsilon^{-\alpha x/2} e^{-c_\varepsilon^{-x}/2}, \quad (25)$$

where the function ϕ is a solution of the confluent hypergeometric equation

$$z\phi'' + (b - z)\phi' - a\phi = 0, \quad (26)$$

with coefficients $b = 1 + \alpha$, $a = (b - \nu)/2$ which are also functions of U . Solution to equation (26) is of the form

$$\phi(z) = C_1 \mathcal{M}(a, b; z) + C_2 \mathcal{U}(a, b; z) \quad (27)$$

where $\mathcal{M}(a, b; z)$ is the Kummer function, and $\mathcal{U}(a, b; z)$ is the Tricomi function, [1]. Finally, the solution of (16) with the potential (24) can be written as

$$\psi(x) = H_\varepsilon(x)[C_1 \mathcal{M}(a, b; c_\varepsilon^{-x}) + C_2 \mathcal{U}(a, b; c_\varepsilon^{-x})]. \quad (28)$$

Proposition 2.3. *For the quantum hydrodynamic model (10)-(11) with $p(n) = 0$ and the boundary conditions (9), with the Morse potential (24), the current-voltage characteristic, $J = J(U)$, is given by*

$$J(U) = \frac{\sqrt{2}}{\Gamma(a)} \frac{1}{H_\varepsilon(0)H_\varepsilon(1)} \frac{\sin(U/\varepsilon)}{[\mathcal{M}(1)\mathcal{U}(c_\varepsilon^{-1}) - \mathcal{U}(1)\mathcal{M}(c_\varepsilon^{-1})]}, \quad (29)$$

for $U \in [0, U_{max}^\varepsilon]$, where $U_{max}^\varepsilon = (1 - c_\varepsilon^{-1})(3 + 2\sqrt{2} - c_\varepsilon^{-1})/4$. Moreover,

$$J(U) \rightarrow 0, \text{ as } U \rightarrow 0 \quad \text{and} \quad J(U) \rightarrow 0, \text{ as } U \rightarrow U_{max}^\varepsilon,$$

Proof. We begin with the formula for current density $J = \varepsilon \operatorname{Im}(\bar{\psi}(0)\psi'(0))$. With the formula (28) we get

$$\begin{aligned} \psi'(x) &= H'_\varepsilon(x)[C_1 \mathcal{M}(a, b; c_\varepsilon^{-x}) + C_2 \mathcal{U}(a, b; c_\varepsilon^{-x})] \\ &\quad - \frac{\sqrt{2}}{\varepsilon} c_\varepsilon^{-x} H_\varepsilon(x)[C_1 \mathcal{M}'(a, b; c_\varepsilon^{-x}) + C_2 \mathcal{U}'(a, b; c_\varepsilon^{-x})]. \end{aligned}$$

Direct calculation gives

$$\varepsilon \operatorname{Im}(\bar{\psi}\psi') = -\sqrt{2}c_\varepsilon^{-x} H_\varepsilon^2(x) \operatorname{Im}(\bar{C}_1 C_2) W(\mathcal{M}(a, b; c_\varepsilon^{-x}), \mathcal{U}(a, b; c_\varepsilon^{-x})).$$

Considering that the Wronskians of the Kummer and Tricomi functions can be written in terms of the Gamma function:

$$W(\mathcal{M}(z), \mathcal{U}(z)) = \mathcal{M}(z)\mathcal{U}'(z) - \mathcal{M}'(z)\mathcal{U}(z) = -z^{-b}e^z/\Gamma(a),$$

we get

$$J = \varepsilon \operatorname{Im}(\bar{\psi}\psi') = \frac{\sqrt{2}}{\Gamma(a)} \operatorname{Im}(\bar{C}_1 C_2). \quad (30)$$

To calculate the complex-valued constants C_1 , C_2 , we use the boundary conditions $\psi(0) = 1$ and $\psi(1) = e^{iU/\varepsilon}$. In this way we obtain the following linear system for C_1 and C_2 :

$$\psi(0) = H_\varepsilon(0)[C_1\mathcal{M}(a, b; 1) + C_2\mathcal{U}(a, b; 1)] = 1,$$

$$\psi(1) = H_\varepsilon(1)[C_1\mathcal{M}(a, b; c_\varepsilon^{-1}) + C_2\mathcal{U}(a, b; c_\varepsilon^{-1})] = e^{iU/\varepsilon},$$

with solution given by:

$$C_1 = \frac{1}{H_\varepsilon(0)H_\varepsilon(1)} \frac{\mathcal{U}(c_\varepsilon^{-1})H_\varepsilon(1) - \mathcal{U}(1)e^{iU/\varepsilon}H_\varepsilon(0)}{\mathcal{M}(1)\mathcal{U}(c_\varepsilon^{-1}) - \mathcal{U}(1)\mathcal{M}(c_\varepsilon^{-1})},$$

$$C_2 = \frac{1}{H_\varepsilon(0)H_\varepsilon(1)} \frac{-\mathcal{M}(c_\varepsilon^{-1})H_\varepsilon(1) + \mathcal{M}(1)e^{iU/\varepsilon}H_\varepsilon(0)}{\mathcal{M}(1)\mathcal{U}(c_\varepsilon^{-1}) - \mathcal{U}(1)\mathcal{M}(c_\varepsilon^{-1})}.$$

Direct calculation gives

$$\operatorname{Im}(\bar{C}_1 C_2) = \frac{1}{H_\varepsilon(0)H_\varepsilon(1)} \frac{\sin(U/\varepsilon)}{[\mathcal{M}(1)\mathcal{U}(c_\varepsilon^{-1}) - \mathcal{U}(1)\mathcal{M}(c_\varepsilon^{-1})]}. \quad (31)$$

Note that

$$H_\varepsilon(0) = e^{-1/2}, \quad H_\varepsilon(1) = c_\varepsilon^{-\alpha/2} e^{-c_\varepsilon^{-1}/2}.$$

By inserting the expression (31) in (30) we finally get (29).

We point out that $J(U)$ depends on U only through the terms $\Gamma(a)$ and $H_\varepsilon(1)$. Let us consider first the case $U \rightarrow 0$:

$$\nu(U) = \frac{2U}{1 - c_\varepsilon^{-1}} + \frac{1}{2}(1 + c_\varepsilon^{-1}) \rightarrow \frac{1}{2}(1 + c_\varepsilon^{-1}), \quad \alpha = \sqrt{2\nu - 1} \rightarrow c_\varepsilon^{-1/2},$$

$$a = \frac{1}{2}(1 + \alpha - \nu) \rightarrow \frac{1}{4} + \frac{c_\varepsilon^{1/2} - 1}{2c_\varepsilon} > 0.$$

The values of $\Gamma(a)$ and $H_\varepsilon(1)$ remain finite in the limit $U \rightarrow 0$ and then, due to $\sin(U/\varepsilon) \rightarrow 0$ we get $J(U) \rightarrow 0$ as $U \rightarrow 0$. Next, consider the case $U \rightarrow U_{\max}$. Then $\nu(U)$ and $\alpha(U)$ converge monotonically to $\nu(U_{\max})$ and $\alpha(U_{\max})$ but $a(U_{\max}) = \frac{1}{2}(1 + \alpha(U_{\max}) - \nu(U_{\max})) \rightarrow 0$. We find that $H_\varepsilon(1)$ remains finite with $U \rightarrow U_{\max}$, but $\Gamma(a)$ is unbounded in the limit $U \rightarrow U_{\max}$. Consequently, $J(U) \rightarrow 0$ when $U \rightarrow U_{\max}$. \square

3. The influence of the pressure term on JU-curve

When treating the QHD model with the pressure term, the explicit expression for the JU curve cannot be obtained, so we discretized the corresponding Schrödinger equation using finite differences and obtained the JU curve numerically. With respect to Madelung's equivalence between the Schrödinger equation and the QHD system, we start with the following nonlinear Schrödinger equation:

$$-\frac{\varepsilon^2}{2}\psi_{xx} + [V(x) + f(|\psi|^2)]\psi = 0 \quad \text{on } (0, 1), \quad (32)$$

with boundary conditions (9). We note that a simple application of the Browder-Minty theorem for monotone nonlinear operators [13] yields that the equation (32) with boundary conditions (9) has a unique weak solution, for f nonnegative and monotonically increasing, considering that $V(x) \geq 0$ on $(0, 1)$. More precisely, using the notation $\psi = u + iv$, $\mathbf{u} = (u, v)$, we rewrite the complex equation (32) as a real system:

$$-\frac{\varepsilon^2}{2}u_{xx} + [V(x) + f(|\mathbf{u}|^2)]u = 0, \quad -\frac{\varepsilon^2}{2}v_{xx} + [V(x) + f(|\mathbf{u}|^2)]v = 0,$$

on $(0, 1)$ with boundary conditions

$$u(0) = 1, \quad u(1) = \cos(U/\varepsilon), \quad v(0) = 0, \quad v(1) = \sin(U/\varepsilon). \quad (33)$$

We define a weak problem as follows: find $\mathbf{u} = (u, v) \in H^1(0, 1) \times H^1(0, 1)$, satisfying the boundary conditions such that

$$\int_0^1 \left(\frac{\varepsilon^2}{2}(u_x \phi_x + v_x \psi_x) + [V(x) + f(|\mathbf{u}|^2)](u\phi + v\psi) \right) dx = 0,$$

for all $(\phi, \psi) \in H_0^1(0, 1) \times H_0^1(0, 1)$. We note that the variational formulation for all locally bounded functions $f: [0, \infty) \rightarrow \mathbb{R}$ and $V: [0, 1] \rightarrow \mathbb{R}$ is well defined due to the embedding of $H^1(0, 1) \subset L^\infty(0, 1)$.

Let us define operator $\mathcal{A}: H_0^1(0, 1) \times H_0^1(0, 1) \rightarrow H^{-1}(0, 1) \times H^{-1}(0, 1)$,

$$\langle \mathcal{A}\mathbf{w}, \mathbf{v} \rangle = \int_0^1 \left(\frac{\varepsilon^2}{2}\mathbf{u}_x \cdot \mathbf{v}_x + [V(x) + f(|\mathbf{u}|^2)]\mathbf{u} \cdot \mathbf{v} \right) dx$$

where $\mathbf{u} = \mathbf{w} + \mathbf{G}$ and $\mathbf{G} = (1 + x(\cos(U/\varepsilon) - 1), x \sin(U/\varepsilon))$. Monotonicity and coercivity of the operator \mathcal{A} follow directly from the assumption that the function f is monotonically increasing and nonnegative, and $V(x) \geq 0$. Namely, let $\mathbf{w}, \mathbf{z} \in H_0^1(0, 1) \times H_0^1(0, 1)$ and $\mathbf{v} = \mathbf{z} + \mathbf{G}$. The direct calculation gives $\langle \mathcal{A}\mathbf{w} - \mathcal{A}\mathbf{z}, \mathbf{w} - \mathbf{z} \rangle \geq \alpha \|\mathbf{w} - \mathbf{z}\|_{H_0^1(0, 1)^2}^2$, where $\alpha = C_P \varepsilon^2 / 2$ and C_P is the constant from the Poincaré inequality. On the other hand, the coercivity follows from the estimate

$$\begin{aligned} \langle \mathcal{A}\mathbf{w}, \mathbf{w} \rangle &= \int_0^1 \left(\frac{\varepsilon^2}{2}|\mathbf{w}_x|^2 + \frac{\varepsilon^2}{2}\mathbf{G}_x \cdot \mathbf{w}_x + [V(x) + f(|\mathbf{u}|^2)](\mathbf{w} + \mathbf{G}) \cdot \mathbf{w} \right) dx \\ &\geq \frac{\varepsilon^2}{2} \int_0^1 |\mathbf{w}_x|^2 dx - C \int_0^1 |\mathbf{w}_x| dx + \int_0^1 [V(x) + f(|\mathbf{u}|^2)](|\mathbf{w}|^2 - |\mathbf{G}||\mathbf{w}|) dx, \end{aligned}$$

where $\mathbf{w} \in H_0^1(0,1) \times H_0^1(0,1)$ and $\mathbf{u} = \mathbf{w} + \mathbf{G}$. Under the assumptions on f and $V(x)$, for sufficiently large $\|\mathbf{w}\|_{H_0^1(0,1)^2}$ the last integral is positive and the coercivity then follows from the Poincaré inequality. In this way we have proved the following existence theorem:

Theorem 3.1. *Let the function $f: [0, \infty) \rightarrow \mathbb{R}$ be nonnegative and nondecreasing and $V(x) \geq 0$ a bounded potential. Then the equation (32) with boundary conditions (9) has a unique solution.*

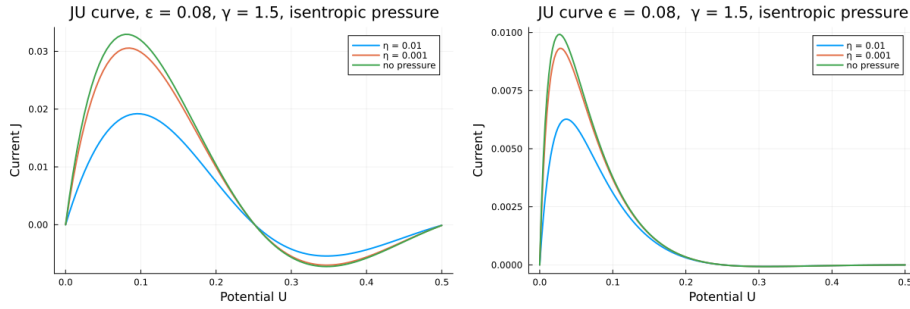


FIGURE 1. The JU-curve for system (10)-(11). Left: the monomial potential, right: the Morse potential. The curves show the NDR effect and the influence of the pressure term on the shape of the JU-curves.

To discuss the numerical results for JU curves for the QHD model with the pressure term, we discretize the problem (32), (9) using the finite differences. To consider the influence of the pressure term in the isentropic case, we assume that the enthalpy function f is scaled with a parameter η , and we consider the behavior of the current-voltage curves when η increases from zero (no pressure case). Figure 1 shows the JU curve resulting from the monomial potential $V(x) = x^m U$, $m = 3$ and the Morse potential. Comparing the JU curve for the QHD model with and without pressure, our simulations show that the pressure term strongly affects the peak-to-valley ratio of the JU curves. The peak of the JU curves decreases compared to the no-pressure case when the η parameter is increased. In summary, our numerical results show that the convexity of the enthalpy function f strongly affects the peak-to-valley ratio of the JU-curves, as shown in Figure 1.

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