

New nonlinear structures in a degenerate one-dimensional electron gas

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Abstract

The collective dynamics of nonlinear electron waves in an one-dimensional degenerate electron gas is treated using the Lagrangian fluid approach. A new class of solutions with a nontrivial space and time dependence is derived. Both analytical and numerical results demonstrate the formation of stable, breather-like modes, provided certain conditions are meet. For large amplitude of the initial density perturbation, a catastrophic collapse of the plasma density is predicted, even in the presence of the quantum statistical pressure and quantum diffraction dispersive effects. The results are useful for the understanding of the properties of general nonlinear structures in dense plasmas.

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I. INTRODUCTION

The collective dynamics of electrons in one-dimensional (1D) nanostructures opens up many new interesting avenues for research because of its application in modern nanotechnology [1, 2]. A 1D geometry can be created from a two-dimensional electron gas at a cleaved or gated heterojunction [3, 4]. The dynamics is qualitatively different when the charge carriers are confined in 1D channels or wires, because then the electrostatic interaction is stronger than in higher dimensions. In fact, new collective excitations arise in 1D. This is the case e.g. for plasmons in pyroelectric-semiconductor composites [5]. The response of electrons confined to one-degree of freedom exhibits exotic phenomena like spin-charge separation and the emergence of correlated-electron insulators [6, 7]. The spin-charge separation phenomenon supports electron charge density and spin density waves. In a different context, nowadays we have an increasing ability to control plasma-fabricated metal-based nanostructures into 1D plasmonic devices [8]. The consideration of quantum effects in such ultra-small systems is becoming increasingly unavoidable. In addition, the target normal sheath acceleration [9] arising from high intensity laser-matter interaction gives an example of dense 1D plasmas, specially with the development of coherent brilliant X-ray radiation sources [10]. However, the associated self-consistent electronic states are highly nonlinear in nature [11, 12]. Therefore, the sensible analytic modeling of strongly localized structures at nanoscale is of considerable interest.

In a multi-dimensional electron gas, numerical simulations predict solitonic structures, when the electron wave packet interacts with the metal surface. These stable structures are formed due to the balance between the electron density-metal surface interactions induced nonlinearity and the wave dispersion [13]. Periodic nonlinear structures appear in magnetized quantum plasmas too [14].

In this Letter, we present for the first time a nonlinear quasi-collapsing analytical solution in the realm of 1D electron waves described by a quantum hydrodynamic model. The electron density can become singular at a finite time due to the strong effectiveness of the Coulomb interaction in 1D. Therefore, under certain circumstances to be specified later, the Fermi pressure and tunneling effects are shown to be unable to prevent the electron density collapsing. For definiteness, the focus will be in metallic nanostructures, although the results apply to a much broader class of systems.

In metallic nanostructures, the thermodynamic temperature is orders of magnitude smaller than the Fermi temperature T_F , hence the equation of state for a degenerate electron gas is indicated. Moreover, the electron-electron collision time scale $\sim 10^{-10}s$ is typically much larger than the plasmon oscillation time scale $\sim 10^{-16}s$, justifying the neglect of collision terms [15, 16] in a first approximation. Nevertheless, the gross features of the electron dynamics in e.g. metal clusters can be described using fluid models, as found from comparison with numerical simulation of more expensive models involving e.g. the Boltzmann equation or density functional theory [17–19].

The hydrodynamic equations describing the 1D electron gas can then be written as

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x}(nu) = 0, \quad (1)$$

$$mn \left(\frac{\partial}{\partial t} + u \frac{\partial}{\partial x} \right) u = -enE - \frac{\partial p}{\partial x} + \frac{\hbar^2 n}{2m} \frac{\partial}{\partial x} \left(\frac{1}{\sqrt{n}} \frac{\partial^2}{\partial x^2} \sqrt{n} \right), \quad (2)$$

and

$$\frac{\partial E}{\partial x} = 4\pi e(n_0 - n), \quad \frac{\partial E}{\partial t} = 4\pi enu, \quad (3)$$

where n, u, m and $-e$ are resp. the electron number density, fluid velocity, mass and charge, while E is the electric field, \hbar is the reduced Planck's constant and n_0 is the bulk ionic density background. The RHS of Eq.(2) contains the quantum statistical pressure $p = mv_F^2 n^3 / (3n_0^2)$, where $mv_F^2/2 = \kappa_B T_F = \hbar^2 (3\pi^2 n_0)^{2/3} / (2m)$ is the Fermi energy, with κ_B being Boltzmann's constant. For instance [16] with $n \sim 10^{28} m^{-3}$ we get $T_F \sim 5 \times 10^4 K$, much larger than the room temperature, justifying the equation of state for a fully degenerate 1D electron gas. The third term $\sim \hbar^2$ in the RHS of Eq. (2) is the Bohm potential due to quantum diffraction. For metallic nanostructures the quantum statistical pressure and the Bohm potential are of the same order [19], so both contributions will be retained. Finally, for simplifying reasons, exchange-correlation as well as non-ideal, collisional effects are left for future work.

Next we present a procedure to derive exact solutions of Eqs. (1) - (3) by using the Lagrangian fluid variables method. We will see how this method can handle the “difficult” nonlinearities represented by the convective $u\partial_x u$ and Bohm potential terms in the momentum equation. In a different context, Lagrangian variables have been considered [20] to the treatment of the wave-breaking problem in quantum plasmas.

We first transform from Eulerian variables (x, t) to Lagrangian variables (ζ, τ) , such that $\zeta = x$ at $t = 0$, where $\tau \equiv t$ and $\zeta \equiv x - \int_0^\tau d\tau' u(\zeta, \tau')$, so that ζ is a function of both x

and t . In terms of the new variables, the material derivative $\partial/\partial t + u\partial/\partial x = \partial/\partial\tau$. Thus, from Eq. (1) we obtain $n(\zeta, \tau)/n(\zeta, 0) = \partial\zeta/\partial x$, where $n(\zeta, 0)$ represents the initial ($\tau = 0$) electron density. The fluid equations, in these variables, are

$$\frac{\partial}{\partial\tau} \left(\frac{1}{n} \right) = \frac{1}{n(\zeta, 0)} \frac{\partial u}{\partial\zeta} \quad (4)$$

and

$$\begin{aligned} \left(\frac{\partial^2}{\partial\tau^2} + \omega_p^2 \right) u = & \frac{\partial}{\partial\tau} \left\{ \frac{-2\kappa_B T_F}{mn_0^2} \frac{n^2}{n(\zeta, 0)} \frac{\partial n}{\partial\zeta} + \right. \\ & \left. + \frac{\hbar^2}{2m^2} \frac{n}{n(\zeta, 0)} \frac{\partial}{\partial\zeta} \left[\frac{1}{\sqrt{n}} \frac{n}{n(\zeta, 0)} \frac{\partial}{\partial\zeta} \left(\frac{n}{n(\zeta, 0)} \frac{\partial\sqrt{n}}{\partial\zeta} \right) \right] \right\}. \end{aligned} \quad (5)$$

The coupled nonlinear partial differential equations Eqs. (4) and (5) are respectively the continuity and momentum equations in the Lagrangian variables. The electric field has been eliminated using the Maxwell equations. Here $\omega_p = \sqrt{4\pi n_0 e^2/m}$ represent the electron plasma frequency.

We seek solutions by separation of variables, assuming $n(\zeta, \tau) = N(\zeta)/\phi(\tau)$ and $u(\zeta, \tau) = U(\zeta)\psi(\tau)$. Inserting into Eqs.(4) and (5) and separating space and time variable equations, we obtain

$$\frac{1}{\psi} \frac{d\hat{\phi}}{d\tau} = \frac{dU}{d\zeta} = C_1, \quad (6)$$

and

$$\begin{aligned} \left(\frac{d(\hat{1}/\phi^3)}{d\tau} \right)^{-1} \left(\frac{d^2}{d\tau^2} + \omega_p^2 \right) \psi(\tau) = & \frac{1}{U(\zeta)} \left\{ -\frac{2\kappa_B T_F}{m} \hat{N} \frac{d\hat{N}}{d\zeta} \right. \\ & \left. + \frac{\hbar^2}{2m^2} \frac{d}{d\zeta} \left(\frac{1}{\sqrt{\hat{N}}} \frac{d^2}{d\zeta^2} \sqrt{\hat{N}} \right) \right\} = C_2, \end{aligned} \quad (7)$$

where $n(\zeta, 0) = N(\zeta)/\phi(0)$, $u(\zeta, 0) = U(\zeta)\psi(0)$ with $\psi(0)/\phi(0) \neq 0$ and where C_1, C_2 are arbitrary constants. Here $\hat{\phi} = \phi/\phi(0)$, $\hat{N} = N/N(0)$, and $N(0)/\phi(0) = n_0$. Eliminating U, ψ between Eqs. (6) and (7) gives the ordinary differential equations

$$\frac{d^2\hat{\phi}}{d\tau^2} + \omega_p^2 \hat{\phi} = \frac{C}{\hat{\phi}^3}, \quad (8)$$

$$\frac{d}{d\zeta} \left(\frac{\hbar^2}{2m^2} \frac{1}{\sqrt{\hat{N}}} \frac{d^2}{d\zeta^2} \sqrt{\hat{N}} - \frac{\kappa_B T_F}{m} \hat{N}^2 \right) = C\zeta. \quad (9)$$

where the separation constant appear as $C = C_1 C_2$. Note that C has the dimension of time⁻². For simplicity, in this Letter two further integration constants were set to zero in

the derivation. Equation (8) is known as Pinney's equation [21] and is endemic in nonlinear analysis. In the autonomous case as in the present application, it has well known explicit analytic solutions, for instance

$$\hat{\phi} = (1 - \hat{\alpha}^2 \sin^2 \omega_p \tau)^{1/2}, \quad (10)$$

where $\hat{\alpha} = \alpha/\omega_p$. We have used the initial condition $\hat{\phi} = 1$, $d\hat{\phi}/d\tau = 0$ and $d^2\hat{\phi}/d\tau^2 = -\alpha^2$, at $\tau = 0$. In other words, a periodic (cosine-like) initial condition with frequency α have been chosen, where we have taken the separation constant $C = \omega_p^2 - \alpha^2$. The solution (10) gives the temporal part of the density modulation. The parameter $\hat{\alpha}^2$ determines how much energy is transported from the initial source to the electron wave i.e. it measures the amplitude of the initial density perturbation. We need $\hat{\alpha}^2 < 1$ or equivalently $C > 0$ for a well behaved solution. In other words, a collapse will be avoided if the RHS of Eq. (8) is repulsive. Pinney's equation also arise for other quantum plasma problems, like in the case of the quantum Buneman instability [22].

Next we consider the space part. Initially, notice the first $\sim \hbar^2$ term inside the bracket in the LHS of Eq. (9) originate from the kinetic energy term in the Schrödinger equation, while the remaining $\sim T_F$ term contains the Fermi pressure contribution. To rewrite Eq. (9), we use initial conditions $\hat{N} = 1$ and $(\hbar^2/2m\sqrt{\hat{N}})d^2\sqrt{\hat{N}}/d\zeta^2 = -\epsilon$ at $\zeta = 0$. Here ϵ is the quantum kinetic energy at $\zeta = 0$. Also the parameter ϵ serves as a measure of the dispersive effects, since it originates from the quantum diffraction term. Integrating once, the space part equation now becomes

$$-\frac{\hbar^2}{2m} \frac{d^2\chi}{d\zeta^2} + \left(\frac{1}{2} m a^2 \omega_p^2 \zeta^2 - \epsilon \right) \chi + \kappa_B T_F \chi^5 = 0, \quad (11)$$

where $\chi = \sqrt{\hat{N}}$, $a = \sqrt{1 - \hat{\alpha}^2}$ and $\epsilon = \epsilon + \kappa_B T_F$. The nonlinear-Schrödinger-like equation (11) describe nonlinear oscillations in Lagrangian variables where the anharmonicity is due to the Fermi temperature $T_F \neq 0$. Similar nonlinear equations arise in related areas, e.g. in the analysis of low-dimensional Bose-Einstein condensates confined by harmonic traps [23].

In the Thomas-Fermi approximation, the quantum (Bohm) potential is neglected, which amounts to neglecting the derivative and $\sim \epsilon$ terms in Eq. (11). In this limit, the density profile becomes

$$n_{TF}(x, t) = \frac{n_0}{\sqrt{1 - \hat{\alpha}^2 \sin^2 \omega_p \tau}} \left(1 - \frac{m a^2 \omega_p^2 \zeta^2}{2 \kappa_B T_F} \right)^{1/2}, \quad (12)$$

in the region $ma^2\omega_p^2\zeta^2 \leq 2\kappa_B T_F$, with the density being zero outside this region.

For sufficiently large initial perturbation or ($\hat{\alpha}^2 \rightarrow 1$), the term containing a in Eq. (11) can be omitted. Then for negligible quantum kinetic energy compared to internal energy i.e. for $\epsilon \ll \kappa_B T_F$, for certain carefully chosen initial conditions we obtain the following approximate solution of Eq. (11),

$$n(x, t) = \frac{n_0}{\sqrt{1 - \hat{\alpha}^2 \sin^2 \omega_p \tau}} \left(\frac{\cosh 2\bar{\zeta} - 1}{\cosh 2\bar{\zeta} + 2} \right), \quad (13)$$

where $\bar{\zeta} = (2m\kappa_B T_F/\hbar^2)^{1/2}\zeta$. It is interesting to note that the spatial density profile is like a gray soliton as shown in Fig. 1. The neglect of the restoring harmonic $\sim \zeta^2$ term is, however, valid for a short interval such that $ma^2\omega_p^2\zeta^2 \ll \epsilon$.

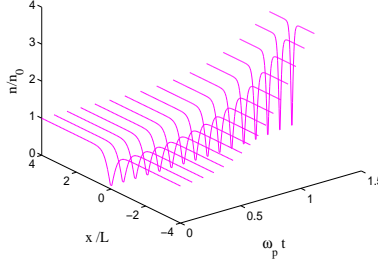


FIG. 1: Normalized density evolution according to Eq. (13), with $\hat{\alpha}^2 = 0.9$ and $\hbar\omega_p/\kappa_B T_F = 0.2$. The length scale is normalized by $L = (\hbar/m\omega_p)^{1/2}$.

It is instructive to examine more closely the exactly resonant case $\hat{\alpha} = 1, a = 0$, for which $\hat{\phi} = \cos \omega_p \tau$ and Eq. (11) reduces to

$$\frac{\hbar^2}{2m} \frac{d^2 \chi}{d\zeta^2} + \epsilon \chi - \kappa_B T_F \chi^5 = 0, \quad (14)$$

which is the equation for an autonomous quintic oscillator. The equation of motion for χ is reducible to quadrature and the exact solution can be expressed in terms of elliptic functions. Indeed, we may rewrite

$$\frac{d^2 \chi}{d\zeta^2} = -\frac{dV}{d\chi}, \quad (15)$$

with the pseudo-potential

$$V = V(\chi) = \frac{\epsilon}{\kappa_B T_F} \frac{\chi^2}{2} - \frac{\chi^6}{6}. \quad (16)$$

From the form of $V(\chi)$ (see Fig. (2)), it follows that periodic motion in the space-like variable ζ appear when the energy integral $(d\chi/d\zeta)^2/2 + V(\chi) < V_{\max}$, where the maximum

value $V_{\max} = (1/3)[\varepsilon/(\kappa_B T_F)]^{3/2}$, and suitable initial value $\chi(0)$ between the turning points. The energy integral can be also used to produce the aforementioned quadrature. A simple analysis of the energy conservation law associated to (15) shows that necessary conditions for nonlinear bounded oscillations are given by $\chi^2(0) < [\varepsilon/(\kappa_B T_F)]^{1/2}$ and $[(d\chi/d\bar{\zeta})(0)]^2 < (2/3)[\varepsilon/(\kappa_B T_F)]^{3/2}$, which is interpreted as follows. The quantity $\chi(\bar{\zeta})$ and the derivative are related to density perturbations and can not be too large, otherwise the diffusive effects due to the Bohm potential and the degeneracy pressure will predominate. On the other hand, a sufficient high ε (or, a sufficiently high restoring electric force related to the plasma frequency ω_p) tends to enlarge the phase space region for which oscillatory motion is possible. Notice, however, that in the exact resonance case treated here the solution will develop a singularity in a finite time since $\hat{\phi} \rightarrow 0$ as $\tau \rightarrow (\pi/2)\omega_p^{-1}$. In this context, the localized solution (13) can be shown to correspond to separatrix motion, in the border between periodic and aperiodic trajectories.

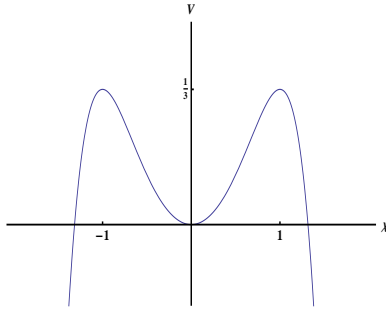


FIG. 2: Pseudo-potential from Eq. (16), with $\varepsilon = \kappa_B T_F$ so that $V_{\max} = 1/3$.

In yet another case, when the internal energy is negligible in comparison with the quantum kinetic energy i.e. $\kappa_B T_F \ll \varepsilon$, Eq. (11) becomes formally identical to the time-independent Schrödinger equation for the simple harmonic oscillator, in Lagrangian coordinates. The solution is in terms of the Hermite polynomials H_ν , with eigenvalues $\varepsilon = \varepsilon_\nu = a\hbar\omega_p(\nu + \frac{1}{2})$, where $\nu = 0, 1, 2, \dots$. More explicitly, disregarding more involved forms involving linear combinations of the elementary solutions, in the limit of negligible Fermi temperature we get

$$n(x, t) = \frac{n_0}{\sqrt{1 - \hat{\alpha}^2 \sin^2 \omega_p \tau}} H_\nu^2 \left[\left(\frac{am\omega_p}{\hbar} \right)^{1/2} \zeta \right] \exp \left(-\frac{am\omega_p}{\hbar} \zeta^2 \right). \quad (17)$$

Figure (3) show the space-time behavior of the density n given by (17) for parameters $\hat{\alpha}^2 = 0.9$ and $\nu = 0$. A quasi-collapse is seen by the blowing up of n just before $t_c = (\pi/2)\omega_p^{-1}$. The spatial width of the density appear as a pulsating breather form after transforming back to Eulerian variables. Multi-breather solutions can be obtained for $\nu = 1, 2, 3...$

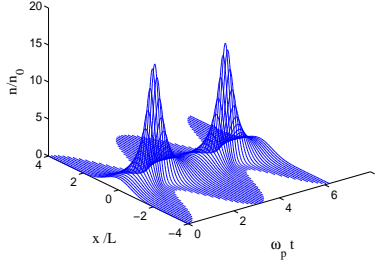


FIG. 3: Normalized density evolution according to Eq. (17), with $\hat{\alpha}^2 = 0.9$ and $\nu = 0$. The figure shows that for $\hat{\alpha}^2 \rightarrow 1$ the density goes towards quasi-singularity in the absence of Fermi temperature. The length scale is normalized by $L = (\hbar/am\omega_p)^{1/2}$.

In the above approximate solutions, the relation between ζ and x is $x = \zeta(1 - \hat{\alpha}^2 \sin^2 \omega_p \tau)^{1/2}$. Furthermore, the fluid electron velocity $u(\zeta, \tau) = -\hat{\alpha}^2 \omega_p \zeta \sin \omega_p \tau \cos \omega_p \tau / (1 - \hat{\alpha}^2 \sin^2 \omega_p \tau)^{1/2}$. Equations represent in limit cases the solution of Eq. (11) in three different physical situations. The parameter $\hat{\alpha}^2$ stands for the strength of the nonlinearity and controls the amplitude of the density modulations. At the time $\tau = (\pi/2)\omega_p^{-1}$, one finds that for $\hat{\alpha}^2 \rightarrow 1$ there appears a quasi-density singularity. Actually $\hat{\alpha} \sim 1$ gives the resonance condition $\alpha \sim \omega_p$. At this resonance, the initial periodic source pumps the maximum energy into the system, resulting in an inward cavitation blowing up the density and shrinking the inhomogeneity width.

Finally, we numerically simulate Eqs. (10) and (11) using a finite difference scheme. The density profile is shown in Fig. (4) for $\hat{\alpha}^2 = 0.9$, total energy parameter $\varepsilon/a\hbar\omega_p = 5.0$ and internal energy parameter $\kappa_B T_F/a\hbar\omega_p = 1.0$. Close to collapse the density becomes strongly peaked and narrow, remaining finite. Increasing the internal energy up to $\kappa_B T_F/a\hbar\omega_p = 5.0$ substantially reduces the density amplitude and finally stable breather structures are formed as shown in Fig. (4). The reduction in density amplitude is attributed to the dispersive effect caused by the quantum statistical pressure. For larger value of the total energy parameter $\varepsilon/a\hbar\omega_p = 9.0$ with $\kappa_B T_F/a\hbar\omega_p = 1.0$, a multi-breather structure for the density is developed

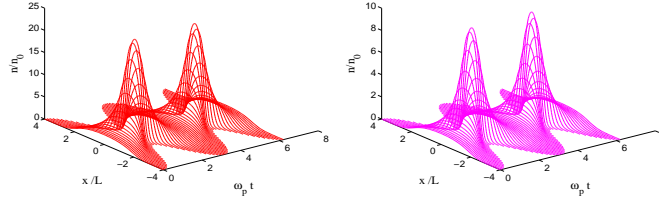


FIG. 4: Normalized density evolution with $\hat{\alpha}^2 = 0.9$. The left-hand side figure shows that for $\varepsilon/a\hbar\omega_p = 5.0$ and $\kappa_B T_F/a\hbar\omega_p = 1.0$ the density tends to a singularity. Increasing the value of $\kappa_B T_F/a\hbar\omega_p = 5.0$, the right-hand side figure exhibits the reduction of the density amplitude and spatial dispersion due to the degeneracy pressure. The spatial variable x is normalized by $L = (\hbar/am\omega_p)^{1/2}$.

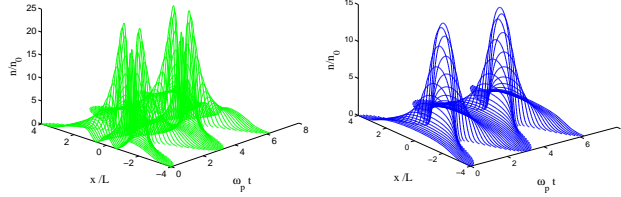


FIG. 5: The left side figure shows the electronic density for $\varepsilon/a\hbar\omega_p = 9.0$, $\kappa_B T_F/a\hbar\omega_p = 1.0$. A multi-breather structure in space and time appear for a small electron Fermi temperature. In the right, a bigger Fermi temperature so that $\kappa_B T_F/a\hbar\omega_p = 4.0$ produce a single breather solution. The length scale is normalized by $L = (\hbar/am\omega_p)^{1/2}$.

in space. However, for higher Fermi temperature (or, higher internal energy) $\kappa_B T_F/a\hbar\omega_p = 4.0$, the multi-breather structure reduces to a single breather, which is depicted in Fig. (5). This is because the restoring harmonic term $\sim \zeta^2$ in Eq. (11), which produces oscillations arising from the initial density perturbations, is overcome by the nonlinearity due to the degeneracy pressure.

In conclusion, we have demonstrated a new route to generate nonlinear electron waves in a fully degenerated 1D electron gas, using Lagrangian variables. The nonlinear structures are described by ordinary differential equations, in significant reduction in comparison to the spatio-temporal fluid equations. Although the focus of the work was on the density oscillations, similar conclusions can be derived for the electric field and quantum fluid velocity. In the limit of large amplitude initial density perturbations (i.e. nearly the resonance $\hat{\alpha}^2 \rightarrow 1$), the plasma density develop a quasi-singular cavitation in finite time. However, the

catastrophic collapse can be avoided for specific parameters allowing the formation of stable breather structures, thanks to the Fermi pressure and Bohm potential contributions. With respect to the stability, the robustness of the new analytical solutions has been numerically verified. On one hand the new stable, long-lived coherent nonlinear structures can be useful for information transport at nanoscales. On the other hand, the derived analytical estimates are useful tools for the determination of the necessary parameters to avoid collapse in real systems. As a general rule, the use of Lagrangian variables in the context of quantum fluid equations is a very promising new avenue for quantum hydrodynamic equations arising in different fields, like the metallic nanostructures considered here, quantum plasmas [24], graphene, plasmonics, or quantum diodes [25], whenever quantum fluid equations are applicable. Further effects, such as dissipation and exchange-correlation energies can significantly change the behaviors found here, but are outside the scope of the present work.

Acknowledgments

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