Publication III


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I. INTRODUCTION

The discovery of the quantum Hall (QH) effect at Landau level filling factor \( \nu = \frac{5}{2} \) in the two-dimensional (2D) electron gas (2DEG) (Ref. 1) marked evidence that incompressible states may form at unusual even-denominator filling fractions. After years of subsequent theoretical and experimental work\(^2\)\(^-\)\(^5\) it is well established that one of the most plausible theoretical candidates for a QH state at \( \nu = \frac{5}{2} \) is an exotic state of matter, a paired quantum Hall state. Since electron-electron (e-e) interactions are repulsive this pair formation is a collective phenomenon involving residual interactions of composite particles that, in this state, are composites of an electron and two vortices. The electron pairing would be analogous to the formation of Cooper pairs in superconductors, although it would be purely a result of e-e interactions without contribution from phonons or other fields. In some theoretical models, the excitations of the paired electron state are predicted to have non-Abelian statistics that could be used in the field of topological quantum computing.\(^2\) In this paper we introduce our theoretical model of QDs in Sec. II and the computational methods used to solve the many-body problem in Sec. III. The exact diagonalization method is used in Sec. IV to calculate the overlaps of the Pfaffian wave function with the exact many-body state. In Sec. V, we analyze the electronic structure of fragmented QH states and show that the second-lowest Landau level (LLL) is spin polarized due to the lifting of degeneracy of single-particle states near the Fermi level. In Sec. VI, we present experimental evidence for fragmentation of QH states in the \( 2 \leq \nu \leq \frac{5}{2} \) filling-factor regime. Section VII concludes our work with discussion of the relevance of QH states in the 2DEG.
of our findings with the observed fragility of the $\nu = \frac{5}{2}$ QH state in disordered or confined 2DEG.

II. MODEL

QDs formed in the GaAs/Al$_x$Ga$_{1-x}$As heterostructure are modeled for both lateral and vertical QD devices as droplets of electrons in a strictly 2D plane confined by a parabolic external potential.\(^10\) We use an effective-mass Hamiltonian

$$H = \sum_{i=1}^{N} \left(\frac{\mathbf{p}_i^2}{2m^*} + V_c(r_i)\right) + \frac{e^2}{4\pi\epsilon_{\text{vac}}\sum_{i<j} r_{ij}},$$

where $N$ is the number of electrons, $V_c(r) = m^*\omega_0^2r^2/2$ is the external parabolic confinement, $m^* = 0.067m_e$ is the effective mass, $\epsilon = 12.7\epsilon_0$ is the dielectric constant of the GaAs semiconductor medium, and $A$ is the vector potential of the homogeneous magnetic field $B$ perpendicular to the QD plane. The confinement strength $\omega_0$ in the calculations is 2 meV, unless otherwise stated.

If the e-e interactions are excluded, the single-particle solutions of Hamiltonian (1) are Fock-Darwin states.\(^15\) In the limit of a very high magnetic field, the Landau level structure approaches that of the 2DEG. However, in finite magnetic fields the external potential alters the electronic structure and different Landau levels overlap. Therefore, the concept of Landau level filling needs to be generalized to finite-size systems. Kinaret et al.\(^16\) defined the average filling factor as $\nu_{\text{ave}} = \frac{N}{2}(N+L)/2$, where $L$ is the total angular momentum. Another possibility is to focus on the LLL and define filling factor of a state as $\nu_{\text{LLL}} = \frac{2N}{N_{\text{LLL}}}$. These definitions differ in the high filling-factor regime, but this is not critical to the interpretation of results that are based on the structural properties of the many-body states.

III. COMPUTATIONAL MANY-BODY METHODS

The ground state corresponding to interacting electrons in QH droplets is solved numerically using the exact diagonalization (ED), density-functional theory (DFT), and the variational quantum Monte Carlo (QMC) method. Since the paired electron state in the 2DEG is a strongly correlated many-body state, the ED method is used to analyze its stability in the QD confining potential. The DFT and QMC methods are used to analyze the fragmented QH states. The regime where this fragmentation gives characteristic signals in the experiments is beyond the reach of the ED method. However, we find that both the DFT and QMC methods provide accurate results in this regime (see the Appendix).

A. Exact diagonalization

In the ED method, we assume that the electrons occupy states on one Landau level only. If we now take a fixed number of states from this Landau level, our computational task is first to construct the many-body basis. Then the Hamiltonian matrix corresponding to Hamiltonian of Eq. (1) is constructed in this basis. Finally, the lowest eigenstate and eigenvalue are found by matrix diagonalization. More details can be found, e.g., in Ref. 17. In addition to the standard Coulomb interaction, we use in the ED two modifications of it. To model the finite thickness of the sample, we use a softened potential\(^18\) defined as

$$V_f(r) = \frac{e^2}{4\pi\epsilon\sqrt{r^2 + d_f^2}},$$

where $d_f$ is the sample thickness. Electrons in second or higher Landau levels move on top of background charge of lower Landau levels, which effectively screens the Coulomb interaction. This is modeled with a screened potential that is of the Gaussian form

$$V_g(r) = \frac{e^2\exp(-r^2/d_s^2)}{4\pi\epsilon r},$$

where $d_s$ is the screening length. The unit of length in our ED results is given by $l = \sqrt{\hbar/m^*\omega}$, where $\omega = \sqrt{\omega_0^2 + (\omega_c/2)^2}$ and $\omega_c = eB/m^*$ is the cyclotron frequency of electron in magnetic field $B$.

B. Density-functional theory

Our DFT approach is based on spin-DFT, a variant of the conventional DFT generalized to deal with nonzero spin polarization. On top of standard spin-DFT, we include the bare external vector potential $A$ [see Eq. (1)] in the Kohn-Sham equation. In contrast with current-spin-DFT, however, we neglect the exchange-correlation potential $A_{\text{xc}}$. In the magnetic-field range considered here, this has been shown to be a very reasonable approximation.\(^19\) As another valid approximation, we neglect the dependence of the exchange and correlation on the vorticity.\(^20\) The exchange and correlation energies and potentials are calculated using the 2D local spin-density approximation, for which we use the QMC parametrization of the correlation energy by Attaccalite et al.\(^21\)

The DFT approach is implemented on a 2D real-space grid and employs a multigrid method for solving of the Kohn-Sham equations.\(^22\) Our symmetry-unrestricted DFT approach has been shown to lead to solutions with broken rotational symmetry that has been linked to mixing of the different eigenstates of angular momentum.\(^23,24\) In a fixed symmetric external potential, this type of spontaneous symmetry breaking is expected to be unphysical. In Sec. VI, we compare the validity of this assumption directly to experimental data.

C. Quantum Monte Carlo

Since the fragmentation of many-body state in the vicinity of $\nu = \frac{5}{2}$ is a delicate many-body problem, we employ the QMC method to analyze the reliability of our DFT approach. The wave function in the QMC is chosen to be

$$\Psi = D_1D_2 \prod_{\nu < j} J(r_{ij}),$$

where the two first factors are Slater determinants for the two spin types and $J$ is a Jastrow two-body correlation factor. The Slater determinants are constructed from the Fock-Darwin states. For the two-body Jastrow factor, we use a form

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\[ f(r) = \exp \left( \frac{Cr}{a + br} \right), \]  

where \( a \) is fixed by the cusp condition to be three for a pair of equal spins and one for opposite ones, and \( b \) is an additional parameter different for both spin-pair possibilities. The ground state of the QD in the spin-droplet regime is calculated assuming that the LLL and the SLL are compact. This means that the Slater determinants are built from single-particle states having angular momenta \( l=0, \ldots, N_{\text{LLL}},-1 \) for spin \( s=\uparrow, \downarrow \) in the LLL and \( l=-1, \ldots, N_{\text{SLL}},-2 \) for the spin \( s \) in the SLL. Energy for each combination of non-negative total spin \( S \) and total angular momentum \( L \) is then calculated. The QMC method deals with the correlation effects in the many-particle system more accurately than the DFT approach. However, the computational cost of the QMC method is significantly larger than that of the DFT. A detailed description of the QMC method is given in Ref. 25.

IV. PFAFFIAN STATE IN QUANTUM DOTS

The structure of the QH states in the 2DEG at half-integer filling factor has been a topic of intense research efforts. Currently, it is regarded plausible that the experimentally observed \( \nu=\frac{5}{2} \) state consists essentially of a full spin-compensated LLL and a half-filled spin-polarized SLL, in which weak \( p \)-wave electron pairing takes place. Formally, the SLL is described by a Moore-Read, or Pfaffian, wave function lifted to the SLL. There exists some theoretical evidence that the excitations of this QH state obey non-Abelian statistics. The ED calculations have become standard tests of trial wave functions of QH states, and they have shown high overlaps with the Pfaffian wave function in the 2DEG. However, there are other candidates for the \( \nu=\frac{5}{2} \) state, some of which possess only Abelian quasiparticle excitations.

The structure of the \( \nu=\frac{1}{2} \) state in QDs was analyzed with the ED method in Ref. 11. Here we provide results for half-filled higher Landau levels with more realistic interelectron potentials defined in Sec. III. Following the theory of the \( \nu=\frac{5}{2} \) QH state in the 2DEG, we assume that the half-filled Landau level is spin polarized. The Pfaffian wave function, which describes paired fermion states of the half-filled Landau level, is defined for LLL as

\[ \Psi_{\text{PF}} = \text{Pr} \left( \frac{1}{z_i - z_j} \right) \prod_{i<j} (z_i - z_j)^{2} \exp \left( -\frac{1}{2} \sum_i r_i^2 \right). \]  

In higher Landau levels the Pfaffian state is obtained by applying the Landau level raising operator to each electron. The angular momentum of the Pfaffian state is \( L' = N' (N' - 1) - (n_{\text{LLL}} + \frac{1}{2}) N' \), where \( N' \) denotes the number of electrons in the half-filled Landau level and \( n_{\text{LLL}} = \{0, 1, \ldots\} \) is the Landau level index.

We present the overlaps of the Pfaffian wave function with the ED eigenstate for electrons frozen to lowest (LLL), second (SLL), or third (TLL) Landau level, which correspond to filling fractions of \( \nu=\frac{5}{2}, \frac{3}{2}, \text{ and } \frac{1}{2} \), respectively. Electrons in the half-filled second and third Landau levels move on top of the uniform background electron density of the spin-compensated lower Landau levels. This background charge effectively screens the Coulomb interaction. In QDs, the e-e interactions are further screened due to metallic leads.

Figure 1 shows the overlaps of the Pfaffian wave function and the ED eigenstate of Coulomb interaction for particle numbers 4 \( \leq N' \leq 12 \). For large particle numbers, the overlaps in the second Landau level are highest. This shows that \( \nu=\frac{5}{2} \) has the highest probability to be described by the Pfaffian.

Next, we study how the screening of the e-e interaction and finite thickness of the sample change the overlaps of the ED eigenstate with the Pfaffian. For six electrons on LLL, the overlaps are slightly improved when the screening and finite sample thickness are taken into account in the interaction (see Fig. 2). On SLL, screening slightly improves the overlap, but a finite thickness lowers it. The same trends can be seen in Fig. 2 for eight electrons, but now the effects are clearly stronger, and there is a large increase in the overlaps.

The highest overlaps are on the order of 0.8–0.9 at \( \nu=\frac{5}{7} \), which means that the structure of the many-body state is close to the Pfaffian. The exact state at the given angular momentum would therefore show electron pairing to a significant degree. We note that the Pfaffian wave function in Eq. (6) has no adjustable parameters. It is possible to modify the Pfaffian wave function by introducing a pairing function that differs from \( g = 1/(z_i - z_j) \) of the Moore-Read form. This would not change the angular momentum of the state but has been found to increase overlaps significantly in the 2DEG.

In addition to the overlaps, it is crucial to verify that the state at the angular momentum of the Pfaffian state is ener-
the half-filled Landau level, respectively, using \( \nu = 1 \) and \( \nu = 3 \) corresponding to \( \nu = 1 \) and \( \nu = 3 \), respectively. The corresponding energy splitting is about 1.5 meV at \( L = 0 \). In comparison, the Zeeman splitting is about 0.05 meV.

FIG. 3. (Color online) (a) Kohn-Sham energy spectrum of a 60-electron quantum dot as a function of single-particle angular momentum \( L \) calculated from the density-functional theory with spin-compensated orbitals. The density of states of the SLL is high near the Fermi energy \( E_F \). The magnetic field is 2.125 T which corresponds to a filling factor of \( \nu = \frac{5}{2} \). (b) The corresponding energy spectrum from spin-density-functional theory shows lifting of the degeneracy near the Fermi level via complete spin polarization of the SLL. The LLL remains spin compensated. Spin \( \uparrow (\downarrow) \) corresponds to spin orientation parallel (antiparallel) to the magnetic field. The spin splitting due to many-body effects is about 1.5 meV at \( L = 0 \). In comparison, the Zeeman splitting is about 0.05 meV.

V. FRAGMENTED QUANTUM HALL STATES

In quantum Hall droplets, single-particle states within each Landau level are not degenerate due to the confining potential. The average distance of an electron from the center of the droplet and therefore also the potential energy increase with angular momentum. This suggests that a compact occupation structure may be energetically favorable. The compact occupation of Landau levels leads to fragmentation of charge and spin densities into incompressible integer filling factor domains. We call these states fragmented quantum Hall states that are alternatives to the paired electron state at half-integer Landau level fillings.

We analyze the structure of fragmented QH states near \( \nu = \frac{5}{2} \) in a harmonic confining potential of a semiconductor quantum dot with the QMC and the DFT methods. The Kohn-Sham single-particle energy spectrum of the Landau levels calculated with the spin-compensated DFT and the spin-DFT are shown in Figs. 3(a) and 3(b), respectively. The spin-DFT and the QMC show that the degeneracy of the single-particle states close to the Fermi energy is lifted via a complete polarization of the second-lowest Landau level. Therefore, a compact occupation of the single-particle states of the spin-compensated LLL and spin-polarized SLL leads to a fragmented state with \( \nu = 2 \) region (double-occupied LLL) at the edges of the droplet and \( \nu = 3 \) (spin-polarized SLL) at the center (Fig. 4).

The spin splitting of the SLL in the spin-DFT calculations is analogous to the Stoner criterion, which states that in the presence of correlations between electrons of the same spin...
and high density of states near the Fermi level, the system prefers ferromagnetic alignment that reduces the degeneracy.\textsuperscript{32} We call the incompressible spin-polarized droplet of SLL electrons a spin droplet.\textsuperscript{12} The size of the spin droplet becomes significant when the number of electrons in the dot \( N \geq 35 \). The nonuniform filling-factor structure of the spin-droplet states is reminiscent of the incompressible QH domains that form in the 2DEG with long-range disorder.\textsuperscript{13} The compact occupation of the SLL leads to a lower angular momentum than what is needed for a paired electron state as described by the Pfaffian wave function (6). For example, the size of the spin droplet in the QMC method is \( N' = 8 \) electrons at \( N = 48 \), and the angular momentum of the SLL is \( L' = 20 \), which can be contrasted to \( L' = 44 \) for the Pfaffian wave function with the same number of electrons.

The SLL remains polarized and compact between \( \nu = 2 \) and \( \nu = 2 \). Hence, we call this filling-factor range the spin-droplet regime. The size of the spin droplet gradually shrinks with the increasing magnetic field as the electrons are passed from the SLL to the LLL. The contributions of the LLL and SLL occupancies to the electron and spin densities are shown in Fig. 4 for the case of 60-electron QD. Qualitatively similar results were obtained for confinement strengths 1–4 meV and electron numbers \( N \) between 35 and 120, which confirm the generality of the results. The calculations show that the energy benefit from the polarization of the SLL is large (see Fig. 3 and the Appendix), which would make spin droplets robust in the presence of impurities in samples.

We note that the stability of the fragmented QH states in large QDs (\( N > 30 \)) can be contrasted to the instability of the maximum-density-droplet (MDD) state in the same regime. The MDD state is the totally polarized state corresponding to the \( \nu = 1 \) QH state in 2DEG, and it has been found to be unstable in large QDs with \( N > 30 \) (Refs. 33 and 34).

VI. SIGNATURES OF FRAGMENTATION IN ELECTRON AND SPIN TRANSPORT

The emergence of finite-size counterparts of integer and fractional QH states in QDs gives characteristic signatures in the chemical potentials. Several experimental methods have been developed to measure the chemical potential in a QD via addition of electrons one-by-one into the system. These experimental methods include Coulomb blockade,\textsuperscript{35} capacitance,\textsuperscript{36} and charge detection techniques.\textsuperscript{37} In this work, we use data from electron transport measurements of QDs in the Coulomb and spin-blockade regime.\textsuperscript{34,38} The spacings of the spin and Coulomb blockade peaks correspond to the energy needed to add the \( N \)th electron in the system of \( N - 1 \) electrons, i.e., the chemical potential defined as \( \mu(N, B) = E_{\text{tot}}(N, B) - E_{\text{tot}}(N - 1, B) \).

We calculate the signatures in the chemical potentials associated with the formation of fragmented QH states and compare these to those obtained from the electron transport data in three different QD devices. Two of the experimental samples (samples A and B) are lateral quantum dots on a 60-electron quantum dot. The net spin-up density is due to spin polarization of the second-lowest Landau level.
FIG. 5. (Color online) Ground-state energy of the $N=47$ quantum dot calculated with the density-functional theory for the rotationally symmetric eigenstates of the angular momentum $L$ (blue curve) and for the ground states in the symmetry-unrestricted approach (magenta curve). The corresponding chemical potentials $\mu(N=47\rightarrow48)$ calculated from the theory are shown in the lower panel together with experimental data from a lateral quantum-dot device (sample B). Dashed lines correspond to the boundaries of the spin-droplet regime. The insets show the fragmented spin and charge densities of three of the corresponding states (cf. Fig. 4). The strength of the parabolic confining potential of the quantum dot is $\omega_0=2$ meV in the calculations.

Spin polarization of the leads shows a phase transition in the system where two phases ($\nu=2$ and 3) coexist, and the size of the $\nu=2$ domain increases with the magnetic field. The chemical potential does not continue to rise, but instead, it is oscillating around a constant value until $\nu=2$. This signature can be found in all the experimental samples (see Fig. 6). All electron transport data presented are thus consistent with the theoretical picture that the ground states in the vicinity of $\nu=2$ involve fragmented QH states. We point out, however, that the results are sensitive to the shape of the external potential, and the pairing of the electrons may still occur if the potential is sufficiently homogeneous, e.g., in large QDs, where the second Landau level would acquire higher angular momentum.

Spin polarization of the leads is commonly used to create a current that depends on the orientation of the electron spin, which passes through the device. In the case of the two lateral QDs in our analysis, the electrons enter the QD from spin-polarized magnetic edge states of the 2DEG through tunneling barriers. Coulomb blockade lifts when the energies of the many-body states corresponding to $N$ and $N+1$ electrons are equal. The tunneling current depends then on the coupling between the wave function in the QD and the electronic states in the external leads. The lowest Landau level orbitals are at the edges of the QD, and the coupling is stronger to the leads compared to the second-lowest Landau level orbitals that are close to the center of the QD. Due to polarization of the leads, their coupling to electron states with spin parallel to the external polarization is higher than the coupling of spins antiparallel to the external polarization. This spin dependence in the transport has been shown to lead to a characteristic checkerboard pattern of current densities through QDs. Our DFT results are consistent with such transport currents in the spin-blockade regime (Fig. 7).

The polarization of the SLL in the $2\leq\nu\leq2$ regime would be in contrast to the model presented in Ref. 40. A consequence of this is that the transport current via SLL orbitals should show no checkerboard pattern in this regime since the spins are always parallel to the polarization of the leads. This could be tested with high-accuracy spin-blockade spectroscopy, which would be able to detect small changes in the weak tunneling currents through the SLL orbitals.

FIG. 6. (Color online) Chemical potentials calculated with (a) the density-functional theory and measured from (b) vertical and (c) lateral quantum-dot devices for various electron numbers. Both experiments show the signal associated with the polarization of the second-lowest Landau level at $\nu=5/2$ in the peak position data when $N\geq30$ in agreement with the theoretical result. The confinement strength ranged from 2 to 4 meV depending on the electron number. The data for the vertical device in (b) are courtesy of Kouwenhoven (Ref. 34) and the data for the lateral device in (c) are courtesy of Sachrajda (Ref. 38).

FIG. 7. (Color online) Checkerboard pattern of transport current in density-functional theory (left panel) and spin-blockade experiments (right panel). The lowest current densities correspond to electron transport via states in the second-lowest Landau level, near the core of the quantum dot. The current density in experiments has been amplified in high magnetic fields with a linear function to compensate for the general attenuation of the signal.
VII. FRAGILITY OF THE $\nu = \frac{5}{2}$ QUANTUM HALL STATE

The $\nu = \frac{5}{2}$ state is one of the most fragile QH states. It is observed only in high-mobility 2DEG samples as the paired electron state may break down in the presence of impurities. These induce a nonuniform potential that, in light of results in this work, may lead to its instability. Our findings are thus in line with those obtained by Chklovskii and Lee\textsuperscript{13} who predicted that in the presence of long-range disorder in the 2DEG, incompressible integer filling factor regions that are separated by domain walls. These structures are analogous to the fragmented QH states that we find in QDs. Structures reminiscent of domain walls have been observed with scanning-probe imaging techniques in a perturbed QH liquid.\textsuperscript{44}

Analogous instability of QH states may also occur in other geometries where the electrons are not strictly confined in all directions, such as in high-mobility 2DEG samples in the vicinity of constrictions. One indication of this may be the observed fragility of the $\nu = \frac{5}{2}$ state in narrow quantum point contacts.\textsuperscript{14} Proposed tests\textsuperscript{9} for the non-Abelian properties of quasiparticle excitations of $\nu = \frac{5}{2}$ QH state make use of finite geometries and multiple constrictions to generate interference among tunneling paths. A possible fragmentation of the $\nu = \frac{5}{2}$ QH state close to the boundaries, which would lead to the instability in such geometries, is still an open question that requires further analysis of the effects of the confinement. While recent experiments on the quasiparticle tunneling,\textsuperscript{6} shot noise generated by partitioning edge currents,\textsuperscript{7} and interferometric measurements of QH edge excitations\textsuperscript{8} of the $\nu = \frac{5}{2}$ QH state show results, which are all consistent with the unusual quasiparticle charge $e^* = \frac{1}{3}$ of the paired electron state, the particle statistics of the excitations remains to be confirmed. Possible fragmentation of QH states in narrow constrictions needed for quasiparticle interferometry adds another challenge in this long quest to confirm the possible non-Abelian characteristics of the $\nu = \frac{5}{2}$ state.

To conclude, we have shown theoretical evidence that electron pairing is possible in small QH droplets in quantum dots at $\nu = \frac{5}{2}$, provided that the half-filled Landau level can acquire sufficiently high angular momentum. However, our calculations indicate that in parabolic external confining potentials the paired electron state breaks down leading to fragmentation of charge and spin densities. We find indirect evidence of such fragmentation in several experiments but point out that our results can be tested by direct measurements of the spatial dependence of spin and charge densities in different geometries and experimental setups.

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APPENDIX: ACCURACY OF NUMERICAL METHODS

The electron correlations play an important role in the structure of fractional QH states. To test for the accuracy of the DFT method in the spin-droplet regime, we compare the energies of different spin-polarization states between the DFT and the QMC method. The number of electrons $N=48$. The linewidths in the QMC denote the statistical error in the results. Only the ground state and the $S=0$ state are shown in the DFT result. The strength of the parabolic confining potential of the quantum dot is $\omega_0 = 2$ meV in the calculations.

Both methods show the spin-droplet structure with a comparable energy benefit in the polarization $\delta \approx 0.5$ meV for $S_{\text{max}} = 4$. The QMC method estimates that the maximum size of the spin droplet is $N_{\text{SD}} = 7$ compared to 8 in the DFT. Given the typical statistical error of $\pm 0.05$ meV in the QMC results, the overall agreement between the methods is excellent. This test indicates that the DFT method captures the essential many-body physics of the spin-droplet formation and gives accurate results for the ground states. The DFT method was subsequently used in the calculation of the chemical potentials of large QDs, which can be compared to the transport experiments in the spin-blockade regime.

The DFT method predicts some noncompact states outside the spin-droplet regime, e.g., $L=375$ and $S=7/2$ state as shown in Fig. 5. This state has one spin-down electron in the SLL with $l=0$. Emergence of noncompact states is a manifestation of the degeneracy of the single-particle states near Fermi level. However, they are rare in the DFT and occur only at magnetic fields below the polarization of the SLL. Detailed analysis of these states with the QMC goes beyond the scope of the present work and is left for future research.
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