LLM-augmented Multi-agent System for Trading Behavior Modeling in Coupled Electricity–Carbon Markets

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Abstract—**The deep integration of electricity and carbon markets introduces new challenges for trading behavior modeling, driven by strategic diversity, adaptive agent behaviors, and bidirectional market feedback. Traditional optimization and game-theoretic formulations, which rely on fixed rationality assumptions and static behavioral structures, often fail to capture these dynamics with sufficient fidelity. This paper proposes a large language model (LLM)-augmented multi-agent system (MAS) framework for trading behavior modeling in coupled electricity–carbon markets, where LLMs act as cognitive agents capable of generating context-dependent strategies, interpreting market rules, and responding to evolving system states. The MAS provides a structured environment for interaction among heterogeneous agents, enabling more expressive, adaptive, and interpretable representations of cross-market behaviors. Case studies based on China's coupled electricity–carbon markets demonstrate that the proposed framework can reflect realistic bidding responses, emission-driven adjustments, and market feedback dynamics. This paper also identifies key challenges and outlines future directions including constraint-aware generation to ensure feasibility, structured reasoning and memory to enhance interpretability, and improved computational efficiency to enable scalable MAS deployment.**

Index Terms—**Large language model (LLM), electricity market, carbon market, trading, multi-agent system (MAS).**

I. Introduction

DRIVEN by the goals of carbon neutrality, the energy system is undergoing a rapid transition toward low-carbon development [1], [2]. Among all emission sources, the power sector plays a critical role in the decarbonization process [3]. To jointly optimize resource allocation and emission reduction, electricity and carbon markets are becoming increasingly interconnected. In coupled settings, carbon price signals are implicitly incorporated into electricity market clearing, influencing dispatch decisions and overall market dynamics. This interaction creates a multi-market and multi-objective decision environment, where market participants must simultaneously consider economic efficiency and carbon compliance. Such coupled electricity–carbon markets have been primarily studied under China's evolving market rules [4], yet the framework and insights are also applicable to other systems such as the European Union Emissions Trading System (EU-ETS). Consequently, power producers face significantly increased complexity in strategy design, as they must manage the interdependent objectives, constraints, and trade-offs arising from market coupling.

The coupled electricity–carbon markets exhibit a bidirectional and dynamic coupling relationship, reflected in both price transmission and strategic response behaviors [5]. On one hand, carbon prices are internalized as part of the marginal generation costs for carbon-intensive units, directly shaping their bidding strategies and affecting their chances of being dispatched in the electricity market [6]. On the other hand, generation decisions affect emissions and quota requirements, which in turn influence carbon price trajectories [7]. This coupling mechanism significantly increases the complexity of market decision-making and makes prices more sensitive to policy and demand changes. When policies shift or unexpected events occur, this tightly linked system may cause price fluctuations to spread in unpredictable ways, potentially disrupting market stability and making regulation more difficult [8].

Given the heightened volatility and interdependence within coupled electricity–carbon markets, developing robust models that capture agent heterogeneity, behavioral dynamics, and regulatory feedback has become increasingly critical. However, current modeling approaches still fall short in representing such complexities. Optimization-based models, while effective for centralized planning, often rely on fixed system assumptions and lack the flexibility to capture agent-level adaptation and learning [9]. Game-theoretic models provide insights into strategic competition but typically assume full rationality and complete information, making them less suitable for environments with uncertainty and behavioral diversity [10]. Reinforcement learning (RL) introduces adaptivity but often struggles with convergence, constraint handling,

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and interpretability [11]. These approaches also fail to incorporate diverse contextual signals such as policies or environmental trends. As a result, they offer limited realism for trading behavior modeling or dynamic policy evaluation. A more expressive and adaptive modeling framework is needed to overcome these challenges and support high-fidelity market analysis.

Large language models (LLMs) have emerged as powerful tools for reasoning, language understanding, and strategic decision-making, offering new opportunities for complex system modeling in energy domains [12], [13]. When combined with multi-agent system (MAS), LLMs enable the construction of a novel simulation framework that more accurately captures the dynamic interactions and behavioral complexity of coupled electricity−carbon markets [14]. Within this framework, LLMs serve as cognitive agents capable of generating strategies, interpreting regulatory signals, and integrating domain knowledge through prompting, tool use, and adaptive fine-tuning [15]. MAS provides a structured environment where heterogeneous agents interact, negotiate, and co-evolve under dynamic system constraints [16]. This integration enables a more comprehensive representation of behavioral heterogeneity, strategic adaptation, and system-level feedback, which are difficult to capture with traditional optimization, RL, and game-theoretic models. Building on these advantages, this framework advances market modeling by allowing agents to interpret policy information, represent heterogeneous behaviors, and reduce reliance on predefined assumptions, leading to more interpretable and adaptive simulations.

This paper investigates how LLMs and MAS can be integrated into coupled electricity−carbon markets by reviewing existing work, identifying key limitations, and developing an LLM-augmented MAS framework. The main contributions are as follows.

1) A review of trading behavior modeling in coupled electricity−carbon markets reveals key limitations and highlights the potential of introducing LLMs.

2) An LLM-augmented MAS framework is proposed, in which LLMs act as cognitive decision-making agents to enable context-aware, interpretable, and adaptive trading behavior modeling.

3) A practical modeling setup for coupled electricity−carbon markets is developed, with case studies from China showing that LLM-augmented MAS can reproduce realistic bidding patterns and cross-market responses.

4) Key challenges related to model reliability and practical integration are discussed, along with future directions in trading behavior modeling.

The rest of this paper is organized as follows. Section II reviews coupled electricity−carbon markets and outlines the potential of LLMs. Section III introduces the LLM-augmented MAS framework. Section IV presents the LLM-augmented MAS framework for trading behavior modeling in coupled electricity−carbon markets. Section V provides a case study with experimental results. Section VI discusses key challenges and future directions. Section VII concludes this paper.

II. Coupled Electricity−Carbon Markets and Potential of LLMs

A. Concept of Coupled Electricity−Carbon Markets

With the acceleration of the energy transition, carbon emission constraints have become an important factor shaping electricity market operations. The coordinated operation of coupled electricity−carbon markets has been extensively studied, particularly in the context of China's evolving market reforms. Specifically, "coordination" refers to market participants simultaneously engaging in electricity and carbon trading. Consequently, the joint modeling of coupled electricity−carbon markets has emerged as a key focus in both research and policy formulation, with recent studies further highlighting the game-theoretic evolution and decision optimization of renewable and low-carbon energy systems in similar decarbonization contexts [17]. Coupled electricity−carbon markets form a unified framework where power generators bid in the electricity market while also meeting carbon-trading obligations tied to their emissions. Carbon prices affect bidding and dispatch by changing marginal costs of generators, while the emission structure of the electricity market shapes carbon price dynamics, forming a two-way feedback relationship. A systematic understanding of such coupling mechanisms is vital for carbon pricing design, clean energy investment, and market stability. While this study focuses on China, the proposed framework has potential applicability to other systems such as the EU-ETS with suitable regional adaptations.

B. Overview of Existing Approaches for Modeling

Existing trading behavior modeling approaches for coupled electricity−carbon markets mainly include optimization, game-theoretic, and RL approaches. References [9] and [18] apply optimization approaches emphasizing system-wide efficiency, but the models are usually built under fixed environmental assumptions, which limits their flexibility in capturing evolving market behaviors. References [10], [19], and [20] use game-theoretic approaches that capture strategic interactions but often assume fully rational agents and complete information, making it difficult to represent bounded rationality or uncertainty. References [11] and [21] employ RL approaches that allow adaptive learning within dynamic environments; however, their adaptability is typically confined to fixed state and reward structures, and retraining is required when market rules or objectives change. In summary, while these approaches have made advances in trading behavior modeling, their adaptability remains largely environment-specific, reducing their ability to reflect behavioral shifts under evolving market conditions.

Existing literature exhibits significant research gaps and limitations. First, the adaptability of current approaches remains largely environment-specific, making it difficult to generalize across different market conditions and accurately represent the evolving interactions and heterogeneous behaviors of participants. Second, many existing approaches rely on fixed or simplified decision structures, which constrain their ability to capture behavioral adaptation under changing market mechanisms. This also leads to limited transparency in decision-making, making regulatory interpretation and validation difficult. Third, the generalization capability of these approaches is often restricted by assumptions about market rules, data availability, and equilibrium structures, which reduces robustness when applied to new policy or operational contexts. Collectively, these limitations highlight the need for a new modeling approach that integrates dynamic adaptability, interpretability, and cross-scenario generalization to better represent evolving market behaviors and system-level interactions in coupled electricity−carbon markets.

C. Potential of LLMs

LLMs have demonstrated remarkable capabilities in natural language understanding, complex reasoning, and knowledge integration, offering a new approach to address the limitations of conventional modeling approaches. Their primary strength lies in utilizing natural language as a flexible interface for processing heterogeneous information, enabling them to interpret and synthesize insights from diverse sources such as policy documents, market regulations, and historical behavioral data—inputs that are typically inaccessible to traditional numerical models. Through carefully designed prompts, LLMs can simulate heterogeneous agent personas, emulating the bounded rationality and diverse strategic objectives of different market participants, from risk-averse thermal generators to profit-maximizing renewable energy producers. This flexibility eliminates the need for hard-coded behavioral rules, allowing for more realistic and adaptive agent modeling. Furthermore, their inherent ability to generate step-by-step reasoning, often referred to as Chain-of-Thought [22] and Tree-of-Thought [23], provides a transparent window into the decision-making process, significantly enhancing the interpretability of agent behavior compared to opaque models such as deep reinforcement learning (DRL) [24]. The capacity for tool use and function calling allows LLMs to act as a cognitive core that interacts with external simulators, optimization solvers, and data application programming interfaces (APIs). This enables them to ground their reasoning in physical constraints and market rules, and to generate structured, actionable outputs such as price-quantity bids. By integrating these capabilities, LLMs can serve as the cognitive engine for intelligent agents, paving the way for a more expressive, transparent, and scalable simulation framework for complex socio-technical systems such as coupled electricity−carbon markets.

III. LLM-AUGMENTED MAS FRAMEWORK

A. Overview

To simulate the strategic behaviors of power producers in coupled electricity−carbon markets, we propose an LLM-augmented MAS framework. The framework consists of four modules: the agent decision module for bidding strategy generation, the market constraint module for feasibility validation, the market simulation module for sequential market clearing, and the strategic learning module for belief updating. This modular design supports heterogeneous agent modeling and long-term adaptation through iterative interactions, enabling high-fidelity simulation of complex and interdependent market dynamics. An overview of proposed LLM-augmented MAS framework for coupled electricity−carbon markets is shown in Fig. 1.

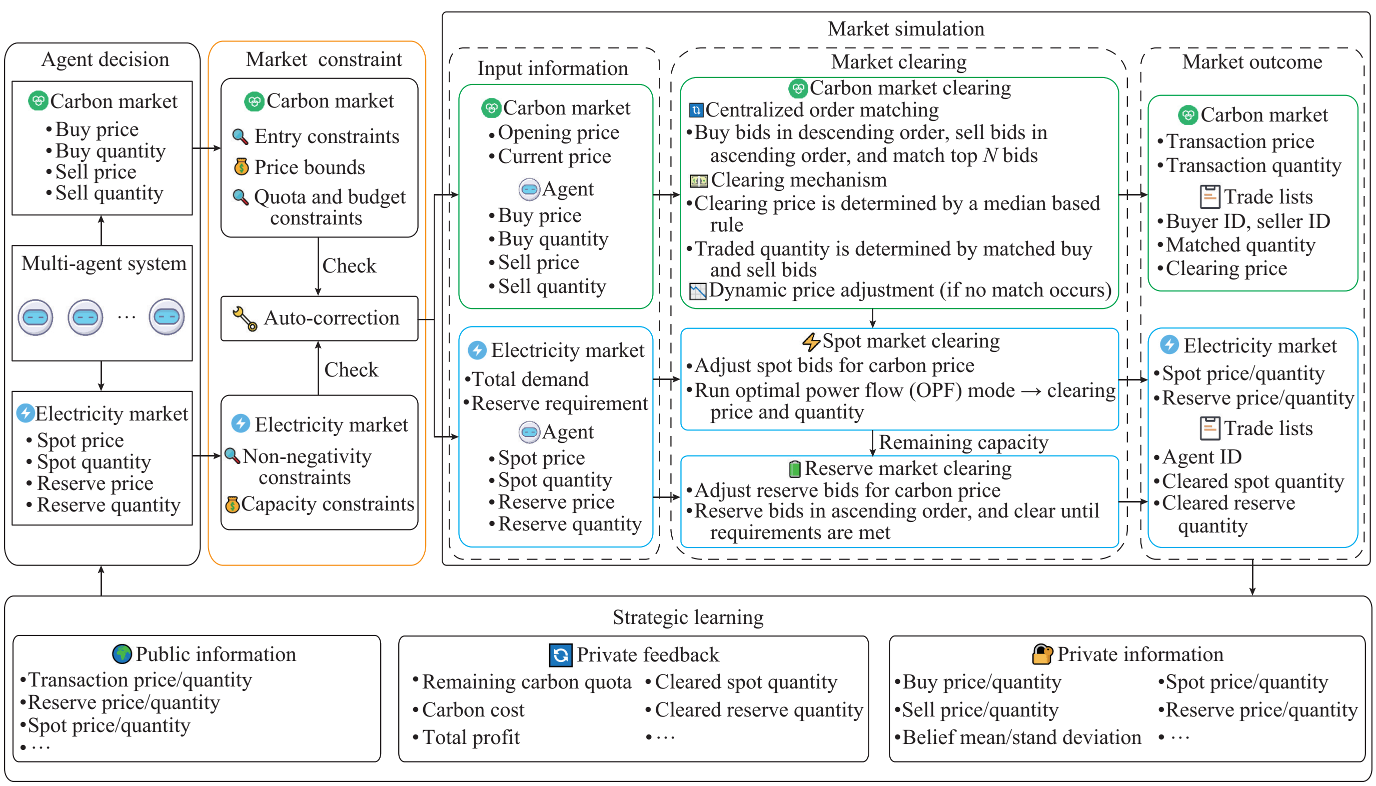

Fig. 1. Overview of proposed LLM-augmented MAS framework for coupled electricity−carbon markets.

Within this framework, each agent is implemented as an LLM-augmented agent, with the LLM serving as its cognitive core. The LLM-augmented agent understands market and policy information, forms decision contexts that integrate public signals and private states, and generates coordinated bidding decisions for the spot, reserve, and carbon markets. These decisions are then passed to the market constraint module to ensure the feasibility of generated decisions. After each clearing process, the LLM updates its internal beliefs based on public information and feedback, supporting iterative and adaptive decision-making in the coupled electricity−carbon markets.

This framework starts with an initialization phase that configures all parameters. These include the number of rounds, electricity demand, reserve requirements, initial carbon prices and quotas, and agent-level attributes such as type, energy cost, reserve cost, capacity, and emission factor, and so on. An initial market state is then constructed accordingly and communicated to all agents in a structured format.

The agent decision module generates bidding strategies by converting multi-source information into structured market actions. Each agent builds a decision context that integrates public signals from electricity and carbon markets with private information such as previous feedback, historical data, and belief states. This context is formatted into a standardized prompt and submitted to the LLM-augmented agent, which then outputs coordinated bidding strategies across electricity, reserve, and carbon markets in the form of price−quantity pairs. The resulting decisions are subsequently forwarded to the market constraint module.

The market constraint module ensures that submitted decisions satisfy explicit constraints in the carbon and electricity markets. The generated bids are evaluated for feasibility with respect to entry constraints, price bounds, and quota and budget constraints of carbon market, as well as non-negativity and capacity constraints of electricity market. Infeasible bids are either automatically corrected or substituted by fallback decisions to maintain system consistency. Only validated decisions are forwarded to the next stage for market simulation module.

The market simulation module sequentially clears the coupled electricity−carbon markets. It first clears the carbon market through centralized bid matching, with the clearing price determined by a median rule. The resulting carbon cost is incorporated into subsequent electricity bids. The market clearing includes spot market clearing and reserve market clearing. Spot market clearing adjusts bids for the carbon price and applies an OPF model to obtain clearing prices and quantities. Given the remaining capacity, reserve market clearing sorts carbon-adjusted reserve bids in ascending bid and clears reserve capacity until reserve requirements are met. This sequential mechanism ensures consistent pricing and coordination across markets, capturing the interdependence between spot market clearing and reserve market clearing.

The strategic learning module updates the cognitive states of agents using market feedback and internal information, enabling continuous adaptation across simulation rounds. By integrating public information, private feedback, and private information, it refines the understanding of market environment for each agent. The updated cognitive states are then passed to the agent decision module as inputs for the next bidding round, forming a closed loop that supports iterative learning and strategic evolution in the dynamic coupled electricity−carbon markets.

B. Agent Decision Module

The agent decision module is responsible for constructing decision context of each agent and generating structured bidding strategies across the carbon and electricity markets. In each round, the agent decision module receives structured inputs from the strategic learning module, forming a comprehensive decision context that integrates public information, private feedback, and private information.

Based on the constructed context, the agent decision module formats a unified prompt using a predefined template, which is output from the strategic learning module, as shown in Fig. 2 and detailed in Section III-E. Within this process, physical and market constraints are explicitly embedded in the reasoning context through structured prompts and constraint-aware environment descriptions, ensuring that most generated strategies satisfy feasibility conditions before market clearing. The prompt is then processed by an LLM to produce structured bidding strategies, returned as explicit price−quantity pairs for the carbon and electricity markets.

You are a rational power producer agent in the coupled electricity−carbon markets, aiming to maximize profit while complying with all market rules and constraints.

You operate as <{role}> (agent ID <{agent_id}>) with a <{technology_type}> generator of <{installed_capacity}> MW and a carbon quota of <{carbon_quota}> tons. Your marginal costs are <{marginal_cost_energy}> CNY/MWh for energy and <{marginal_cost_reserve}> CNY/MWh for reserve. In the previous round, you submitted carbon market buy and sell bids at <{buy_price}>/<{buy_quantity}> and <{sell_price}>/<{sell_quantity}>, and electricity market spot and reserve bids at <{spot_bid_price}>/<{spot_bid_quantity}> and <{reserve_bid_price}>/<{reserve_bid_quantity}>. Your belief about competitors is characterized by belief mean <belief_mean> and belief standard deviation <belief_std>.

Private information

In round<{round_number}>, the market environment includes a system load of <{system_load}> MW, reserve requirement <{reserve_requirement}> MW, carbon opening price <{carbon_opening_price}> CNY/tCO$_2$ (bounds <{carbon_price_bounds}>), and network topology <{network_topology}>. The previous-round clearing results include a carbon market price/quantity of <{last_carbon_price}>/<{last_carbon_quantity}>, a spot market price/quantity of <{last_spot_price}>/<{last_spot_quantity}>, and a reserve market price/quantity of <{last_reserve_price}>/<{last_reserve_quantity}>.

Public information

From previous rounds, you have remaining quota <{remaining_quota}>, carbon cost <{carbon_cost}>, cleared spot quantity <{cleared_spot_quantity}>, cleared reserve quantity <{cleared_reserve_quantity}>, and total profit <{total_profit}>.

Private feedback

Follow the market rules: <{market_rules}>, and ensure bids are feasible and within limits. Based on the above, generate your bidding strategy in the following JavaScript object notation (JSON) format.

Fig. 2. Example of a prompt template from strategic learning module to agent decision module.

The generated strategies constitute the output of the agent decision module and are forwarded to the market constraint module for feasibility validation. The agent decision module thus enables each agent to dynamically adapt bidding behavior in response to evolving market conditions through LLM-augmented strategic reasoning.

C. Market Constraint Module

The market constraint module is responsible for validating the feasibility of submitted bids and enforcing critical operational constraints before market simulation module. It checks compliance across both the carbon and electricity markets, including entry constraints, price bounds, and quota and budget constraints of carbon market, as well as non-negativity and capacity constraints of electricity market. All bids must pass this verification stage to qualify for market clearing.

When violations are detected, the market constraint module applies predefined auto-correction rules. Invalid entries may be discarded or rejected, negative values are reset to zero, and bids exceeding capacity or budget limits are proportionally scaled down to restore feasibility. This correction mechanism ensures physical plausibility and contributes to the stability of multi-agent interactions. The market constraint module acts as a final safeguard to handle rare infeasible cases. As system complexity grows, the proposed framework can integrate external solvers such as OPF or unit commitment (UC) to enhance realism and scalability while maintaining interpretability and feasibility.

The final output of this module is a set of validated and standardized bidding strategies that comply with all operational constraints. These corrected bids are passed to the market simulation module for centralized market clearing across carbon, spot, and reserve markets.

D. Market Simulation Module

The market simulation module is responsible for clearing the carbon and electricity markets, establishing the interaction pathways between them, and generating structured feedback for learning and state updates. The clearing process follows a sequential structure: the carbon market is settled first, providing a carbon price signal, followed by the electricity market, which is further divided into spot and reserve markets. Each sub-process handles the matching of bids and the computation of clearing outcomes. This module ultimately outputs clearing prices, traded quantities, and matched participant information, which serve as critical inputs for belief updates and strategic adaptation of agents.

The carbon market clearing process adopts a price-priority matching mechanism. Constraint-validated buy and sell bids are ranked by price, with buy bids in descending order and sell bids in ascending order. The top N ranked buy and sell bids are matched. Clearing price is determined by a median-based rule. Traded quantity is determined by matched buy and sell bids. If no match occurs, a dynamic price adjustment mechanism is activated in response to observed supply–demand imbalances. The outputs include the updated clearing price, the traded quantity, and the identities of matched agents.

For the spot market clearing, the carbon price signal is systematically accounted for by adjusting the submitted spot bids to reflect emission-related costs, followed by OPF-based clearing. These constraint-validated and adjusted bids, together with system demand and network topology data, constitute the input to the clearing process. As part of the tool use framework (see Fig. 3), the OPF inputs are structured into OPF model matrices, capturing bus data, generator parameters, branch limits, and generation costs. The OPF solver then executes a constrained optimization to minimize total generation cost while satisfying capacity limits, power balance, and transmission constraints. This computational tool ensures that the clearing results respect the physical feasibility of the system and provides spot prices and cleared generation quantities as outputs, which serve as actionable signals for the dispatch decisions of agents.

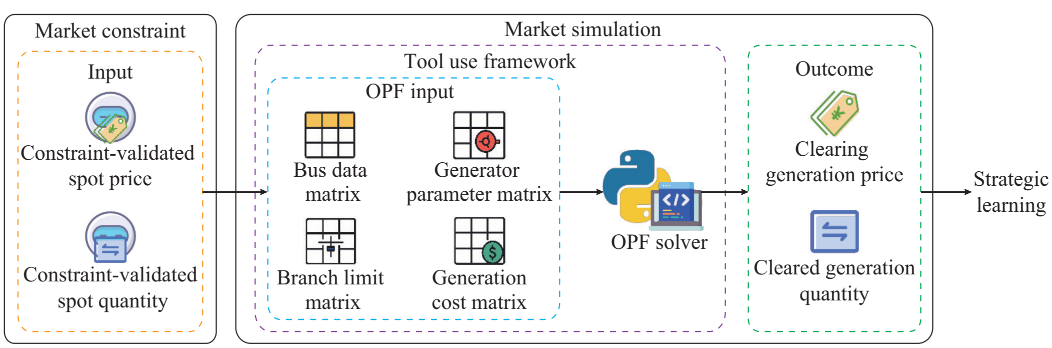

Fig. 3. Market clearing process utilizing tool use framework.

For the reserve market clearing, reserve bids are sorted in ascending bid of price and sequentially accepted until the reserve requirement is satisfied. The module outputs include clearing prices and quantities for both spot and reserve markets, along with agent-specific dispatch results and round metadata.

E. Strategic Learning Module

The strategic learning module constructs and dynamically updates the internal cognitive state of each agent, serving as a central interface that links environmental perception, memory, and policy evolution. In each simulation round, this module processes three categories of input: public information, private feedback, and private information. By integrating these heterogeneous inputs and applying belief update mechanisms, this module infers the cost structures of competitors and supports the generation of bidding strategies that are both strategically aware and environmentally adaptive.

Public information refers to market-wide variables observable by all agents in the current round. It includes transaction prices and quantities in the carbon market, spot prices and quantities, and reserve prices and quantities. These signals form a shared basis for perception of agents of the strategic environment.

Private feedback captures the performance outcomes of agents from the previous round. It includes the remaining carbon quota, carbon cost, cleared spot quantity, cleared reserve quantity, and the total profit. These signals reflect how previous strategies perform and serve as key inputs for belief updates and subsequent decision-making.

Private information reflects the internal reasoning state and long-term behavioral profile of agents. It includes the buy and sell prices and quantities in the carbon market, spot and reserve prices and quantities in the electricity market, as well as belief statistics characterized by belief mean and belief standard deviation over competitors' cost structures. Each belief distribution is characterized by a mean μ_i^t and a standard deviation σ_i. The belief update follows a heuristic rule:

$$\mu_i^{t+1} = \mu_i^t + \alpha_i^t \sigma_i \lambda \tag{1}$$

where λ is a predefined learning rate; and α_i^t is a dynamic adjustment factor of agent i in trading round t, determined by the bid result and its deviation from the clearing price.

This belief update mechanism, inspired by bounded-rational learning principles [25], enables agents to iteratively adjust expectations of competitors' costs based on market feedback. It balances interpretability and efficiency, forming a perception−memory−evolution loop that refines strategies under dynamic market conditions.

To effectively deliver the updated cognitive state to the agent decision module, the strategic learning module formats its outputs into a unified prompt using a predefined template, as shown in Fig. 2. This prompt organizes public information, private feedback, and private information into a coherent and interpretable representation that reflects the strategic perspective of agents. The LLM processes this prompt to generate structured bidding strategies, which are returned as explicit price−quantity pairs for the carbon, spot, and reserve markets. This engineering approach for prompt provides a critical interface that integrates environmental signals, historical outcomes, and internal beliefs into actionable decisions.

IV. LLM-AUGMENTED MAS FRAMEWORK FOR TRADING BEHAVIOR MODELING IN COUPLED ELECTRICITY−CARBON MARKETS

A. Mechanism of Coupled Electricity-Carbon Market

In the proposed framework, two types of transactions are modeled: ① electricity trading, where power producers submit bids for spot and reserve services; and ② carbon allowance trading, where the same producers buy or sell emission allowances based on their emission factors and compliance requirements. Producers act as strategic participants in both markets, and their bidding behaviors are interdependent due to the cost coupling introduced by carbon prices.

To capture this interdependence, a sequential market clearing mechanism is designed. By adopting joint bidding, staged clearing procedures, and coordinated strategy updates, the mechanism allows carbon price signals to influence electricity market outcomes and facilitates strategic consistency across markets [26].

In each trading round t, power producers submit independent bids to the electricity and carbon markets. The carbon market is cleared first to determine the carbon market clearing price λ_{carbon}^t, hereafter referred to as the carbon price. In the subsequent electricity market clearing, the market operator implicitly accounts for the carbon price through an adjustment function applied to the submitted electricity bids. The carbon-adjusted spot offer price $p_{spot\text{-}adj,i}^t$ and reserve offer price $p_{reserve\text{-}adj,i}^t$ used in clearing are given by:

$$p_{spot\text{-}adj,i}^t = f(p_{spot,i}^t, \lambda_{carbon}^t, EF_i) \tag{2}$$

$$p_{reserve\text{-}adj,i}^t = f(p_{reserve,i}^t, \lambda_{carbon}^t, EF_i) \tag{3}$$

where $p_{spot,i}^t$ and $p_{reserve,i}^t$ are the spot and reserve offer prices of producer i in trading round t; and $f(\cdot)$ is the operator's adjustment function incorporating the carbon price λ_{carbon}^t and the emission factor EF_i, ensuring that the electricity market clearing reflects carbon costs.

After incorporating carbon costs, the electricity market jointly clears the spot and reserve markets, allocating cleared spot and reserve quantities $P_{spot,i}^t$ and $P_{reserve,i}^t$ and determining the corresponding spot and reserve market clearing prices λ_{spot}^t and $\lambda_{reserve}^t$. Each producer's profit $Profit_i^t$ is calculated as (4) with the total revenue R_i^t defined in (5) and the total cost C_i^t defined in (6).

$$Profit_i^t = R_i^t - C_i^t \tag{4}$$

$$R_i^t = \lambda_{spot}^t P_{spot,i}^t + \lambda_{reserve}^t P_{reserve,i}^t \tag{5}$$

$$C_i^t = GenCost_i \cdot (P_{spot,i}^t + P_{reserve,i}^t) + \lambda_{carbon}^t (\mathcal{E}_i^t - Q_i^t) \tag{6}$$

where $GenCost_i$ is the marginal generation cost of agent i; $\mathcal{E}_i^t$ is the emission from cleared generation of producer i in trading round t; and Q_i^t is the carbon quota allocated to producer i in trading round t. The term $\mathcal{E}_i^t - Q_i^t$ represents the net carbon obligation, where a positive (negative) value implies a financial cost (revenue).

B. Carbon Market Clearing Mechanism

A centralized bid-matching mechanism is employed to simulate the carbon market clearing process [9]. In each trading round, the system receives buy and sell bids from power producers, represented as quadruples $(q_i^{buy}, p_i^{buy}, q_i^{sell}, p_i^{sell})$, indicating the quantities and prices for intended purchase and sale of carbon allowances. After validating bids, the system performs bilateral matching to determine the carbon price λ_{carbon}^t, executed trade quantities, and updated monetary balances and carbon allowance holdings for each producer.

To ensure feasibility and regulatory compliance, all submitted bids must meet predefined market constraints. First, the submitted buy and sell quantities must be strictly positive:

$$\begin{cases} q_i^{buy} \geq 0 \\ q_i^{sell} \geq 0 \end{cases} \tag{7}$$

Second, the bid prices must lie within an admissible fluctuation range around the previous opening price S, designed to prevent speculative manipulation [9]:

$$p_i^{buy}, p_i^{sell} \in [(1-\delta)S,\ (1+\delta)S] \tag{8}$$

where δ is a predefined fluctuation margin.

Finally, each producer must have sufficient monetary and quota resources to support its bids. The expenditure of a buy bid cannot exceed the available monetary balance, and the quantity of a sell bid cannot exceed the held carbon allowances:

$$\begin{cases} q_i^{buy} p_i^{buy} \leq M_i \\ q_i^{sell} \leq CEA_i \end{cases} \tag{9}$$

where M_i is the available budget of producer i for carbon allowance trading; and CEA_i is the remaining carbon emission allowance of producer i.

In trading round t, the carbon market applies a price−time priority matching rule. Let P_0^t and Q_0^t denote the price and quantity of the lowest-price valid sell bid (with earliest time as a tie-breaker), and P_1^t and Q_1^t denote the price and quantity of the highest-price valid buy bid, respectively. If $P_1^t \geq P_0^t$, a transaction is executed. The traded emission quantity E_i^t is determined as [9]:

$$E_i^t = \min(Q_1^t, Q_0^t) \tag{10}$$

The carbon price λ_{carbon}^t is set as the median of P_0^t, P_1^t, and λ_{carbon}^{t-1} [9]:

$$\lambda_{carbon}^t = median(P_0^t, P_1^t, \lambda_{carbon}^{t-1}) \tag{11}$$

To enhance price discovery under low-liquidity conditions, a dynamic adjustment mechanism is introduced [27]. The market imbalance I^t in trading round t is defined as:

$$I^t = \frac{D^t - S^t}{D^t + S^t} \tag{12}$$

where D^t and S^t are the total demand (buy quantity) and supply (sell quantity) in the carbon market, respectively. This formulation yields a bounded signal in $(-1, 1)$, enabling stable and scale-independent pricing dynamics.

When no direct match occurs under the price−time priority matching rule, or to dynamically adjust the price based on aggregate bid imbalance, the carbon price λ_{carbon}^t is updated using a sensitivity-based rule [28]:

$$\lambda_{carbon}^t = \lambda_{carbon}^{t-1} + \Delta\lambda_{carbon}^t = \lambda_{carbon}^{t-1} + \alpha I^t \lambda_{carbon}^{t-1} + \epsilon^t \tag{13}$$

where $\Delta\lambda_{carbon}^t$ is the incremental price adjustment driven by aggregate bid imbalance in trading round t; α is a sensitivity coefficient; and $\epsilon^t \sim N(0, 0.01\lambda_{carbon}^{t-1})$ denotes the random market shock in trading round t.

After price determination and matching, each participant's account is updated accordingly. For buyer i, the remaining carbon allowance CEA_i^{t+1} and the available budget M_i^{t+1} represent the updated number of held emission allowances and the remaining monetary funds after trading in trading round t:

$$\begin{cases} CEA_i^{t+1} = CEA_i^t + \sum_j E_{i,j}^t \\ M_i^{t+1} = M_i^t - \sum_j \lambda_{carbon}^t E_{i,j}^t \end{cases} \tag{14}$$

where $E_{i,j}^t$ is the amount of carbon allowances purchased by buyer i from seller j at λ_{carbon}^t in trading round t.

C. Electricity Market Clearing Mechanism

The electricity market clearing process is extended to reflect carbon costs, whereby the market operator adjusts both spot and reserve bids based on the carbon price. Specifically, the carbon-adjusted spot and reserve offer prices defined in (2) and (3) are used in clearing, enabling a unified co-optimization framework that incorporates emission costs into market outcomes.

Each producer i must satisfy basic bidding constraints to participate in the market. First, non-negativity is required for both quantities and prices:

$$P_{spot,i}^t, P_{reserve,i}^t, p_{spot-adj,i}^t, p_{reserve-adj,i}^t \geq 0 \tag{15}$$

Second, the sum of submitted spot and reserve quantities cannot exceed the producer's installed capacity C_i, with a tolerance rate τ:

$$P_{spot,i}^t + P_{reserve,i}^t \leq (1+\tau)C_i \tag{16}$$

1) Stage 1: Spot Market Clearing

In trading round t, a centralized OPF model determines the optimal dispatch for each producer by minimizing the total generation cost:

$$\min_{P_{g,i}^t} F = \sum_{i=1}^n f_i\,(P_{g,i}^t) = \sum_{i=1}^n (a_i (P_{g,i}^t)^2 + b_i P_{g,i}^t + c_i) \tag{17}$$

where F is the total generation cost; n is the number of producers; $P_{g,i}^t$ is the power output assigned to producer i in the OPF solution in trading round t; $f_i(\cdot)$ is the generation cost function of producer i, parameterized by a_i, b_i, and c_i; and $P_{spot,i}^t$ is the spot quantity cleared for producer i in trading round t. The optimization is subject to system-level constraints including power balance and generation capacity.

The uniform spot market clearing price λ_{spot}^t is determined by the locational marginal price (LMP) at the reference bus, as shown in (18). The cleared spot quantity $P_{spot,i}^t$ for producer i is given by its dispatched power output in the OPF solution [29], as shown in (19).

$$\lambda_{spot}^t = \left.\frac{\partial \mathcal{L}}{\partial P_d}\right|_{bus=ref} \tag{18}$$

$$P_{spot,i}^t = P_{g,i}^t \tag{19}$$

where $\mathcal{L}$ is the Lagrangian function of the OPF problem; P_d is the system demand; and $bus = ref$ denotes the reference bus at which the LMP is evaluated.

2) Stage 2: Reserve Market Clearing

Following spot market clearing, the residual generation capacity of each producer is used to determine the available reserve $R_{available,i}^t$:

$$R_{available,i}^t = \min(P_{reserve,i}^t, C_i - P_{spot,i}^t) \tag{20}$$

Let $\mathcal{I}=\{1,2,\ldots,n\}$ denote the set of producers. Sort them in the ascending bid of their carbon-adjusted reserve offer prices [30]:

$$p^t_{reserve-adj,1} \le p^t_{reserve-adj,2} \le \ldots \le p^t_{reserve-adj,n} \tag{21}$$

Define the cumulative reserve supply S^t_k under this bid as:

$$S^t_k = \sum_{j=1}^{k} R^t_{available,j} \quad k=1,2,\ldots,n \tag{22}$$

The system reserve requirement in trading round t, denoted as R^t_{req}, is defined by reliability standards. Let j^* be the smallest index such that the cumulative reserve supply equals or exceeds R^t_{req}, which identifies the marginal producer in the reserve market.

$$j^* = \min\{k | S^t_k \ge R^t_{req}\} \tag{23}$$

The cleared reserve quantity for each producer is given as:

$$P^t_{reserve,j} = \begin{cases} R^t_{available,j} & j<j^* \\ R^t_{req} - \sum_{k=1}^{j^*-1} R^t_{available,k} & j=j^* \\ 0 & j>j^* \end{cases} \tag{24}$$

The reserve market clearing price is set by the marginal producer:

$$\lambda^t_{reserve} = p^t_{reserve-adj,j^*} \tag{25}$$

where $p^t_{reserve-adj,j^*}$ is the carbon-adjusted reserve offer price submitted by producer j^*.

V. Case Study

A. Settings

1) Agent Settings

To simulate strategic behaviors in coupled electricity−carbon markets, we configure six representative agents covering coal-fired, gas-fired, energy storage, and renewable energy technologies. Technical and economic parameters are calibrated from authoritative literature and industry standards. Marginal costs for energy range from 230 to 350 CNY/MWh, based on typical operational costs of Chinese thermal power plants and electricity market design principles [31], [32], with reserve costs set at approximately 20% of marginal costs following standard ancillary service pricing practices. Emission factors comply with Intergovernmental Panel on Climate Change (IPCC) [33] guidelines: 0.84-1.05 tCO_2/MWh for coal-fired units, 0.38 tCO_2/MWh for gas-fired units, and near zero for renewable energy and storage systems [34]. Carbon quota allocation follows the baseline method specified in China's national emission trading system [35]. Detailed technical and economic parameters of agents are presented in Table I.

TABLE I
TECHNICAL AND ECONOMIC PARAMETERS OF AGENTS

Agent ID	Type	Capacity (MW)	Marginal cost (CNY/MWh)	Reserve cost (CNY/MWh)	Emission factor (tCO_2/MWh)	Annual quota ($ktCO_2$)
Agent-1	Conventional coal-fired	600	230	46	0.92	1923
Agent-2	Modern CCGT	450	290	45	0.38	676
Agent-3	Large coal-fired for baseload	1000	300	60	0.84	3418
Agent-4	Old coal-fired	300	265	53	1.05	517
Agent-5	Energy storage peaking	200	350	70	0.00	0
Agent-6	Advanced clean energy	500	240	48	0.02	52

Note: CCGT is short for combined cycle gas turbine.

Each agent is equipped with a belief module that represents its internal estimate of the average marginal cost of other producers. The initial belief is modeled as a Gaussian distribution with a mean of 300 CNY/MWh, corresponding to the initial estimate of other producers' average marginal costs of the agent, and a standard deviation of 60 CNY/MWh, where the standard deviation remains fixed throughout the simulation. The belief mean, which captures the current cost estimate of the agent, is updated in each round following a heuristic rule, with a learning rate set to be $\lambda=0.1$. The dynamic adjustment factor α^t_i is determined based on the relationship between the bid of the agent and the market clearing price. Specifically, $\alpha^t_i=1.0$ when the agent clears the market with a bid significantly lower than the clearing price; $\alpha^t_i=-1.0$ when the agent fails to clear the market with a bid higher than the clearing price; $\alpha^t_i=0.2$ when the bid is slightly below the clearing price and the agent successfully clears the market; and $\alpha^t_i=0$ in all other cases.

2) LLM Generation Configuration

To control the generation behavior of the LLM during strategy formation, a set of inference parameters is applied. The model used is Gemini-2.0-Flash. The temperature is set to be 0.3 to ensure low randomness. The LLM module operates in inference-only mode and can be replaced with open-source models that can be locally deployed, ensuring data privacy and deployment flexibility.

3) Market Settings

The simulation of coupled electricity−carbon markets spans 12 monthly rounds representing one operational year. The load profile exhibits a dual-peak seasonal pattern with summer (August, 1640 MW) and winter (January, 1560 MW) peaks, and a spring valley (April, 875 MW), yielding a peak-to-valley ratio of 1.87. With a total installed capacity of 3050 MW, the system maintains an 86% reserve margin, creating a capacity-abundant environment that intensifies market competition. Operating reserves are set at 15% of total load. The electricity market adopts a centralized dispatch mechanism based on DC-OPF, which jointly clears spot and reserve markets under varying load conditions. The carbon market is initialized at 65 CNY/tCO_2 with a price range of 40-150 CNY/tCO_2. When no trades occur, carbon prices are dynamically adjusted using a sensitivity-driven rule with coefficient $\alpha=0.05$ and a maximum adjustment of ±15% per round, ensuring stable yet responsive price formation that reflects supply−demand dynamics.

This study uses a simplified market as a verification case. The proposed framework can be extended to realistic power systems by leveraging the capabilities of LLM-augmented agents, which include system-level context modeling, external tool integration, and constraint consistency verification, to enable high-fidelity simulation and interpretable decision-making.

B. Baseline Comparison and Performance Analysis

To demonstrate the effectiveness of the proposed framework, we develop an RL baseline based on the classical *Q*-learning algorithm [36], which serves as a fundamental baseline in electricity market bidding research and is widely used to benchmark strategic learning methods. The RL baseline employs an expanded 160-state space (8 price levels multiplied by 4 demand levels multiplied by 5 quota levels) and 12 discrete bidding actions, with an adaptive learning rate and a linearly decaying exploration rate from 0.3 to 0. After 1000 training rounds, the RL baseline achieves an annual profit of 1.558×10^9 CNY and annual emissions of 7759 ktCO_2. In contrast, the proposed framework, operating under zero-training conditions, achieves a profit of 1.999×10^9 CNY and annual emissions of 6597 ktCO_2, corresponding to a 28.3% profit increase and a 15.0% emission reduction. These results demonstrate the superior reasoning capability of the proposed framework in optimizing decisions within complex market environments.

C. Carbon Market Simulation Results

To evaluate the effectiveness of the mechanism of coupled electricity−carbon markets, this subsection analyzes the carbon price and trading quantity observed over the 12 monthly rounds, as shown in Fig. 4(a). Carbon prices exhibit an overall upward trend, with modest fluctuations in the early rounds and a continued increase from round 6, increasing from 68.9 CNY/tCO_2 in round 1 to 110.4 CNY/tCO_2 in round 12, with an average level of around 80 CNY/tCO_2. This reflects the growing scarcity of carbon allowances and the rising compliance pressure among agents. Meanwhile, trading quantities remain consistently active, ranging between 113.9 and 150.8 ktCO_2 across all rounds, indicating a stable and liquid market. The overall increase in carbon prices, together with sustained trading activity, demonstrates balanced market dynamics: high-emission units actively purchase allowances for compliance, while low-emission and energy storage units profit from selling surplus quotas. Overall, the results confirm that the mechanism of coupled electricity−carbon markets effectively stabilizes carbon price formation and encourages rational trading responses, capturing the dynamic balance between economic incentives and emission reduction behaviors.

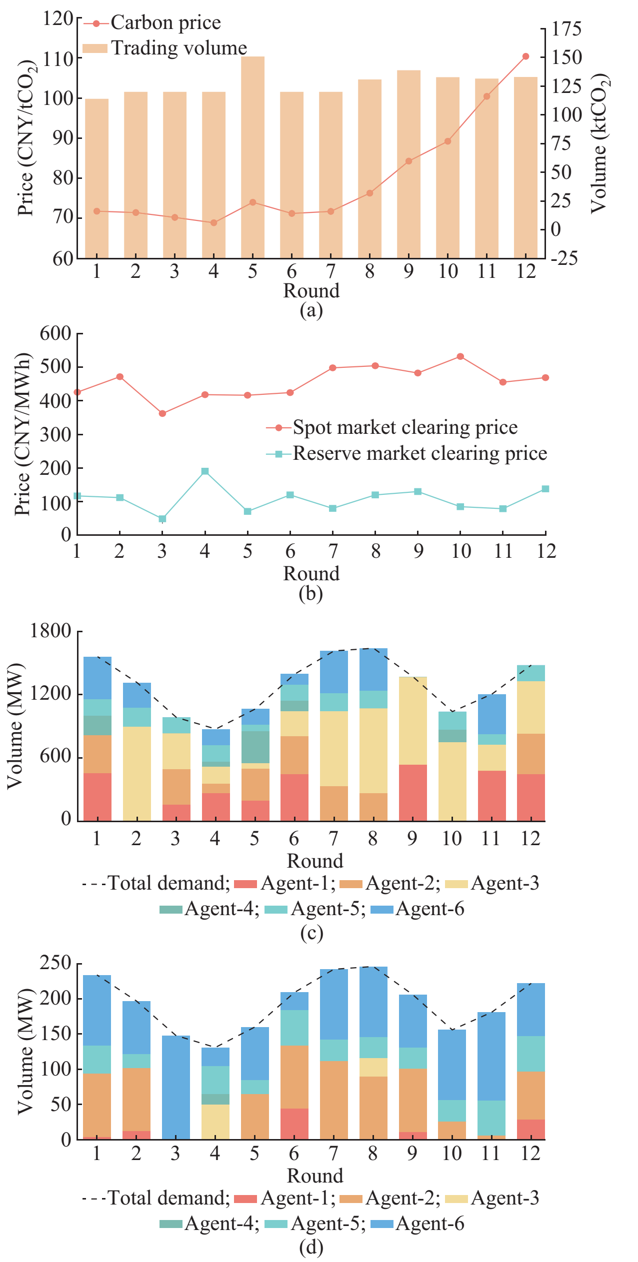

Fig. 4. Simulation results of coupled electricity−carbon markets. (a) Carbon price and trading quantity. (b) Spot and reserve market clearing prices. (c) Spot market dispatch per agent and total demand. (d) Reserve market dispatch per agent and total demand.

D. Electricity Market Simulation Results

The electricity market simulation reveals distinct price dynamics, clearing patterns, and strategic differentiation among agents. Spot and reserve market clearing prices show markedly different temporal behaviors. As shown in Fig. 4(b), the spot market clearing price fluctuates moderately across 12 monthly rounds, ranging from 362.0 to 531.7 CNY/MWh (mean 454.8 CNY/MWh), with a gradual upward trend driven by rising demand and marginal costs. In contrast, reserve market clearing prices vary more sharply between 49.0 and 190.5 CNY/MWh, reflecting stronger sensitivity to system flexibility constraints and bidding concentration.

As shown in Fig. 4(c), the spot market exhibits a moderately concentrated structure, where the top three agents jointly account for 67.9% of total cleared energy, suggesting a competitive yet oligopolistic pattern. Agent-3 dominates energy supply with a share of 35.1%, followed by Agent-1 and Agent-2 with shares of 17.6% and 15.2%, respectively, while Agent-4 participates minimally due to cost disadvantages or strategic withdrawal. The reserve market shows an opposite pattern, as illustrated in Fig. 4(d), dominated by Agent-6 (42.6%), Agent-2 (31.6%), and Agent-5 (17.0%), while the others contribute marginally. This contrast reflects clear strategic differentiation: some agents prioritize energy market dominance, whereas others leverage flexibility to capture reserve revenues.

Overall, the results indicate rational and market-specific positioning. Agent-3 focuses on energy supply leadership, Agent-6 maintains balanced participation, and Agent-2 to Agent-5 display complementary strategies. The centralized dispatch mechanism based on DC-OPF effectively coordinates competition and flexibility, promoting efficient resource allocation and strategic optimization under realistic cost and capability constraints.

E. Coupled Electricity−Carbon Market Simulation Results

To evaluate the economic performance of all agents, Table II summarizes their comprehensive outcomes in the coupled electricity−carbon markets. Here, a positive "allowance gap" indicates a quota shortfall, while a negative value signifies a surplus. Agent-3 achieves the highest net profit of 7.061×10^8 CNY despite the highest annual emissions (3339 ktCO_2), reflecting strong cost competitiveness and an allowance surplus of 79 ktCO_2 that eliminates penalties. Agent-1 ranks second with a net profit of 4.488×10^8 CNY but incurs a penalty of 1.08×10^7 CNY from an allowance shortfall of 72 ktCO_2. Agent-6 ranks third with a net profit of 3.525×10^8 CNY, benefiting from near-zero emissions (32 ktCO_2) and an allowance surplus of 20 ktCO_2. Agent-2 and Agent-5 earn moderate returns with surplus allowances and zero penalties, while Agent-4 has the lowest net profit of 8.60×10^7 CNY, burdened by an allowance shortfall of 47 ktCO_2 and a penalty of 7.0×10^6 CNY.

TABLE II
COMPREHENSIVE OUTCOMES OF AGENTS IN COUPLED ELECTRICITY−CARBON MARKETS

Agent ID	Type	Annual emission (ktCO_2)	Allowance gap (ktCO_2)	Profit (10^8 CNY)	Penalty (10^6 CNY)	Net profit (10^8 CNY)
Agent-1	Conventional coal-fired	1995	72	4.596	10.8	4.488
Agent-2	Modern CCGT	667	−10	2.642	0.0	2.642
Agent-3	Large coal baseload	3339	−79	7.061	0.0	7.061
Agent-4	Old coal-fired	564	47	0.930	7.0	0.860
Agent-5	Energy storage peaking	0	0	1.240	0.0	1.240
Agent-6	Advanced clean energy	32	−20	3.525	0.0	3.525

The results demonstrate that profitability depends on both dispatch competitiveness and carbon compliance. High-emission units remain profitable with cost advantages and effective allowance management, while cleaner technologies benefit from penalty avoidance but require sufficient dispatch. The penalty mechanism (1.78×10^7 CNY in total) effectively internalizes carbon costs, incentivizing operational efficiency and low-emission strategies. The robustness of the proposed framework is further verified by repeating the experiments with different random seeds, yielding an average constraint violation rate of only 1.39%, confirming its reliability in maintaining physical feasibility.

F. Rational Reasoning Mechanism of LLM-augmented Agents

To demonstrate the rational reasoning mechanism of the LLM-augmented agent in the coupled electricity−carbon markets, this subsection takes the decision of Agent-3 in round 3 as an example, and the corresponding core reasoning chain is shown in Fig. 5. The example illustrates how the agent forms a coherent and interpretable decision process based on observable information and cost constraints. The agent first performs market analysis, integrating historical spot, reserve, and carbon prices, together with system demand and reserve requirements, to characterize the current market environment. It then conducts cost analysis by evaluating marginal generation costs in the spot and reserve markets, which defines its feasible operating range. Next, through competitor evaluation, the agent estimates the expected clearing price range by analyzing historical clearing outcomes. Based on these inputs, the agent proceeds to strategy formulation, where it decides whether to submit spot bids below the expected clearing level, whether to participate in or skip the reserve market, and whether to buy carbon allowances for hedging future compliance costs. In the risk assessment, where the agent assesses the trade-off between high bid and risk of non-dispatch, the trade-off between low bid and reduced profit margins, as well as the uncertainty arising from carbon price volatility. Finally, in the final decision, the agent outputs concrete spot, reserve, and carbon trading decisions consistent with the analyzed costs, risks, and market conditions. Compared with traditional rule-based or optimization-based agents, the LLM-augmented agent demonstrates the ability to reason transparently and coherently under observable information and rational expectations, exhibiting superior interpretability and consistency in complex coupled markets.

To examine the rationality and cross-market coordination of agent decisions within the coupled electricity−carbon markets, Agent-3 and Agent-6 are selected as example. The market environment and agent decision logic across operational stages are shown in Table III. The results show that Agent-3 and Agent-6 adaptively coordinate their strategies across the three markets as environment evolves. During the low-load period, they maintain economic operation through flexible adjustments of generation and reserve supply. During the demand recovery period, they develop balanced strategies that consider both profitability and compliance. While during the compliance and peak period, they regulate energy output, respond to reserve requirements, and manage carbon allowances to ensure system stability and policy alignment. Overall, the behavioral evolution of different types of agents aligns with their technical and economic characteristics, demonstrating that the LLM-augmented agents exhibit rational, interpretable, and coordinated decision-making in coupled electricity−carbon markets.

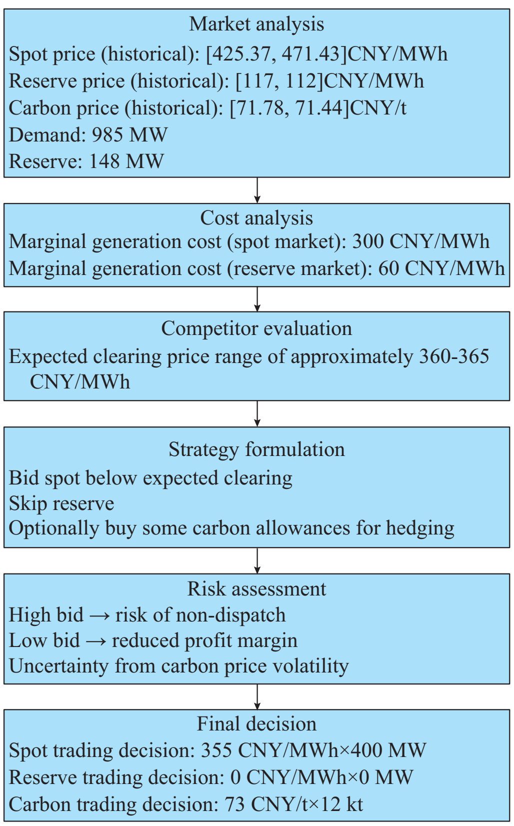

Fig. 5. Core reasoning chain of Agent-3 in round 3.

VI. Key Challenges and Future Directions

A. Key Challenges

The application of LLMs to multi-agent decision-making in coupled electricity−carbon markets raises critical challenges related to physical feasibility, behavioral consistency, and system scalability. These challenges arise because LLMs do not inherently encode engineering constraints, offer limited rationality and interpretability in decision-making, and struggle with the high-dimensional action spaces and computational demands of multi-agent settings. Addressing these limitations is essential to ensure credible, controllable, and scalable LLM-augmented agent behavior in coupled market environments.

1) Lack of Embedded Physical Constraints

LLMs do not natively encode physical laws or system constraints, often producing infeasible or unsafe strategies [37]. Because they reason through linguistic patterns rather than engineering principles, LLMs frequently violate limits on generation, power balance, or operational feasibility. In coupled electricity−carbon markets, such violations become more serious as agents may produce conflicting actions in the electricity and carbon markets at the same time. Post-hoc filtering cannot fully resolve this issue. Addressing it requires integration of constraint-aware generation approaches, external feasibility checkers, or prompt structures explicitly grounded in system rules.

2) Lack of Rationality and Interpretability in Agent Behavior

LLM-augmented agents exhibit unpredictable and non-transparent behaviors, which fundamentally challenge the reproducibility and interpretability of multi-agent decision-making [38]. Unlike traditional agents optimized through explicit objective functions, LLM-augmented agents rely on autoregressive language generation conditioned on prompts. Their decisions are shaped by model architecture, sampling parameters, and implicit statistical patterns learned during pretraining—rather than by symbolic reasoning or domain constraints. This results in a lack of consistent decision logic, making it difficult to trace outputs back to meaningful rules or intentions. As agent behavior becomes highly sensitive to prompt phrasing and internal stochasticity, it resists systematic explanation or control. In the context of coupled electricity−carbon markets, where decisions propagate across agents and market layers, such behavioral variability can distort coordination outcomes and undermine the validity of simulation-based policy evaluations.

TABLE III
Market Environment and Agent Decision Logic Across Operational Stages

Stage (round)	Market environment	Decision logic	
		Agent-3	Agent-6
Low-load period (round 3)	Electricity and carbon markets remain loose with low prices; system load and reserve demand are weak	Operate at low load to maintain base generation, avoid reserve participation, and observe carbon price to minimize compliance risk	Reduce generation, provide reserve capacity for stable income, and sell surplus allowances for liquidity
Demand recovery period (round 7)	Load and prices rise; reserve demand increases; carbon price rebounds from the bottom	Expand generation output to capture profit, reduce participation in the reserve market, and gradually purchase carbon to hedge future compliance cost	Restore mid-high generation, maintain partial reserve supply, and reduce carbon sales to keep compliance margin
Compliance and peak period (round 11)	Electricity and carbon prices remain high; system tightness and compliance pressure intensify	Moderate generation, prioritize compliance, and complete full carbon purchase even with lower profit margin	Sustain high generation and reserve supply, and retain remaining allowances to stabilize market and support policy goals

3) High-dimensional Strategy Spaces and Computational Overhead

LLM-augmented MAS faces scalability bottlenecks due to the combinatorial nature of coupled decision spaces and the high cost of inference. In coupled markets, joint decision-making across interrelated dimensions significantly increases the complexity of the strategy space, which grows exponentially with the number of variables involved. Effective decision-making also requires memory of past states, but LLMs lack long-term memory and are constrained by limited context windows, leading to behavioral inconsistency [39]. Frequent and parallel LLM calls across agents further increase latency and resource usage, making real-time or large-scale deployment impractical. These challenges call for agent architectures equipped with memory compression, shared caching, and more efficient prompting techniques.

B. Future Directions

To address these challenges, future research may consider the following directions, prioritized by their impact on feasibility, interpretability, and scalability. First, ensuring physical feasibility through constraint-aware generation is essential to produce safe and executable strategies. Second, improving interpretability and reasoning consistency requires modular cognitive architectures that structure agent logic. Third, enhancing computational efficiency is key to scaling MAS under realistic resource limits.

1) Constraint-aware Generation and Feasibility Assurance for Power Systems

To address the lack of physical constraint awareness in LLM outputs, future research should aim to improve both the physical feasibility and consistency of generated strategies. Incorporating external feasibility verification modules into the existing LLM-augmented agent framework provides a practical and effective approach. These modules can interface with established power system solvers (e.g., MATPOWER, PandaPower) through Python APIs to perform real-time power flow validation and constraint checking, thereby improving the physical reliability of generated results without altering the model architecture. Building on this foundation, internal constraint-aware generation mechanisms can be further explored, including structured prompting, constraint-conditioned decoding, and feasible-domain encoding, which embed system boundaries such as power flow balance, ramping limits, and carbon quotas directly into the generation process [40]. In parallel, integrating dynamic tool-use capabilities (e.g., solver or rule-checker calls) within the reasoning loop can support real-time compliance monitoring during decision generation [41]. Future work may explore digital-twin-based multi-scenario co-training frameworks, enabling LLMs to interact with simulators and continuously learn system dynamics and thus achieving physically consistent and self-corrective strategy generation.

2) Interpretable and Rational Agent Decision-making

To enhance the interpretability and behavioral rationality of LLM-augmented agents, future research can advance in two directions: internal adaptation and external augmentation. Internally, domain-adaptive fine-tuning on structured market datasets can embed bidding rules, constraint relationships, and operational logic directly into the model, aligning its reasoning process with real market mechanisms and reducing irrational behaviors. Externally, retrieval-augmented generation (RAG) and structured prompting techniques can enable the model to dynamically reference market regulations, historical data, and equilibrium information during inference, generating traceable decision processes based on step-by-step or tree-structured reasoning [42], [43]. These approaches offer a progressive implementation pathway: RAG and structured prompting can be readily integrated into existing simulation frameworks to enhance transparency and explainability; domain-adaptive fine-tuning can further strengthen internal consistency during model training; and the development of hybrid architectures incorporating symbolic reasoning modules may ultimately enable self-explanatory and policy-aligned agent systems, establishing a feasible route toward verifiable decision-making in complex market environments.

3) Resource-efficient Reasoning and Scalable MAS Coordination

In large-scale MAS, LLM inference remains computationally expensive, requiring the development of scalable and resource-efficient deployment strategies. From an implementation perspective, resource-efficient reasoning can be achieved by integrating prompt caching, compressed representations of interaction histories, and parameter sharing among role-specific agents to reduce redundant computation and improve inference throughput [44]. As system complexity increases, hybrid reasoning architectures can be introduced, where LLMs handle high-level strategic reasoning while repetitive or low-level optimization tasks are delegated to RL or symbolic planning modules, effectively mitigating inference bottlenecks without compromising interpretability [45]. In the longer term, scalable MAS coordination can be achieved by distilling frequent subtasks into lightweight policy models that remain semantically aligned with the main LLM, allowing them to handle routine decisions autonomously while maintaining consistent reasoning and scalable coordination across agents.

VII. Conclusion

This paper presents an LLM-augmented MAS framework for capturing the complex dynamics of coupled electricity–carbon markets. Embedding LLMs as cognitive agents allows this framework to generate strategies, model adaptive behaviors, and perform contextual reasoning using historical data and real-time feedback. MAS provides a structured environment for heterogeneous agents to interact, negotiate, and evolve under dynamic constraints. Together, this integration offers significant improvements in expressiveness, interpretability, and system adaptability compared with traditional optimization- or game-theoretic approaches. A prototype implementation is developed to illustrate the ability of the proposed framework to model market clearing, price evolution, and strategic behaviors in realistic multi-agent settings.

Despite its promise, the proposed framework still faces challenges that must be addressed for practical deployment.

Key issues include ensuring the physical feasibility of LLM-generated actions, improving the consistency and interpretability of agent behaviors, and overcoming scalability constraints driven by high-dimensional decision spaces and computational overhead. Future research should therefore focus on constraint-aware generation to enhance feasibility, structured agent architectures to improve interpretability and reasoning consistency, and more efficient mechanisms to support scalable multi-agent execution. Progress in these areas will be crucial for developing the next generation of intelligent platforms that can robustly support market analysis and the transition toward a resilient, low-carbon electricity system.

References

[1] Y. Li, T. Feng, L. Liu *et al*., "How do the electricity market and carbon market interact and achieve integrated development? A bibliometric-based review," *Energy*, vol. 265, p. 126308, Feb. 2023.

[2] X. Yang, B. Cai, and Y. Xue, "Review on optimization of nuclear power development: a cyber-physical-social system in energy perspective," *Journal of Modern Power Systems and Clean Energy*, vol. 10, no. 3, pp. 547-561, May 2022.

[3] M. Yang, Y. Xue, B. Cai *et al*., "Co-optimization of carbon reduction and carbon sequestration in power sector toward carbon neutrality," *Journal of Modern Power Systems and Clean Energy*, vol. 13, no. 5, pp. 1481-1494, Sept. 2025.

[4] W. Liu, J. Zhao, J. Qiu *et al*., "Interpretable hybrid experimental learning for trading behavior modeling in electricity market," *IEEE Transactions on Power Systems*, vol. 38, no. 2, pp. 1022-1032, Mar. 2023.

[5] Q. Ji, D. Zhang, and J. Geng, "Information linkage, dynamic spillovers in prices and volatility between the carbon and energy markets," *Journal of Cleaner Production*, vol. 198, pp. 972-978, Oct. 2018.

[6] B. Lanz and S. Rausch, "General equilibrium, electricity generation technologies and the cost of carbon abatement: a structural sensitivity analysis," *Energy Economics*, vol. 33, no. 5, pp. 1035-1047, Sept. 2011.

[7] T. Niu, H. Li, G. Chen *et al*., "Pricing and distributed scheduling framework of multi-microgrid system based on coupled electricity-carbon market," *Journal of Modern Power Systems and Clean Energy*, vol. 13, no. 3, pp. 1026-1039, May 2025.

[8] X. Zhou, H. Zhao, Y. Cao *et al*., "Carbon market risk estimation using quantum conditional generative adversarial network and amplitude estimation," *Energy Conversion and Economics*, vol. 5, no. 4, pp. 193-210, Aug. 2024.

[9] W. Liu, B. He, Y. Xue *et al*., "A comprehensive modeling framework for coupled electricity and carbon markets," *Energy Conversion and Economics*, vol. 5, no. 1, pp. 1-14, Feb. 2024.

[10] M. Bossy, N. Maizi, and O. Pourtallier. (2014, Aug.). Game theory analysis for carbon auction market through electricity market coupling. [Online]. Available: https://arxiv.org/abs/1408.6122

[11] D. Han, H. Zhang, J. Peng *et al*., "Spatiotemporal optimized dispatch of electric vehicles under electricity-carbon joint market," *IEEE Transactions on Transportation Electrification*, vol. 11, no. 4, pp. 8714-8728, Aug. 2025.

[12] Y. Cheng, H. Zhao, X. Zhou *et al*., "A large language model for advanced power dispatch," *Scientific Reports*, vol. 15, p. 8925, Mar. 2025.

[13] X. Lu, J. Qiu, Y. Yang *et al*., "Large language model-based bidding behavior agent and market sentiment agent-assisted electricity price prediction," *IEEE Transactions on Energy Markets*, *Policy and Regulation*, vol. 3, no. 2, pp. 223-235, Jun. 2025.

[14] T. Guo, X. Chen, Y. Wang *et al*., "Large language model based multi-agents: a survey of progress and challenges," in *Proceedings of the Thirty-third International Joint Conference on Artificial Intelligence*, Jeju Island, South Korea, Aug. 2024, pp. 8048-8057.

[15] T. Schick, J. Dwivedi-Yu, R. Dessi *et al*., "Toolformer: language models can teach themselves to use tools," *Advances in Neural Information Processing Systems*, vol. 36, pp. 68539-68551, Dec. 2023.

[16] Y. Rizk, M. Awad, and E. W. Tunstel, "Decision making in multiagent systems: a survey," *IEEE Transactions on Cognitive and Developmental Systems*, vol. 10, no. 3, pp. 514-529, Sept. 2018.

[17] L. Cheng, F. Yu, P. Huang *et al*., "Game-theoretic evolution in renewable energy systems: advancing sustainable energy management and decision optimization in decentralized power markets," *Renewable and Sustainable Energy Reviews*, vol. 217, p. 115776, Jul. 2025.

[18] L. Wang, C. Yang, Z. Xu *et al*., "Analysis of carbon electricity coupled market modeling method based on carbon credit trading mechanism," *International Journal of Electrical Power & Energy Systems*, vol. 156, p. 109707, Feb. 2024.

[19] L. Wang, Z. Wu, W. Gu *et al*. (2021, Sept.). Hierarchical electricity and carbon trading in transmission and distribution networks based on virtual federated prosumer. [Online]. Available: https://arxiv. org/abs/2109.07213

[20] Y. Zhang, Q. Wu, H. Ren *et al*., "A multi-agent distributed electricity-carbon shared trading strategy considering regional carbon inclusion," *Renewable Energy*, vol. 239, p. 122075, Feb. 2025.

[21] S. Li, P. Wang, X. Zhu *et al*., "Peer-to-peer electricity-carbon coupling trading market based on multi-agent reinforcement learning," in *Proceedings of 2024 IEEE Sustainable Power and Energy Conference*, Kuching, Malaysia, Nov. 2025, pp. 410-415.

[22] J. Wei, X. Wang, D. Schuurmans *et al*., "Chain-of-thought prompting elicits reasoning in large language models," *Advances in Neural Information Processing Systems*, vol. 35, pp. 24824-24837, Dec. 2022.

[23] S. Yao, D. Yu, J. Zhao *et al*., "Tree of thoughts: deliberate problem solving with large language models," *Advances in Neural Information Processing Systems*, vol. 36, pp. 11809-11822, Dec. 2023.

[24] E. ŞAHiN, N. N. Arslan, and D. Özdemir, "Unlocking the black box: an in-depth review on interpretability, explainability, and reliability in deep learning," *Neural Computing and Applications*, vol. 37, no. 2, pp. 859-965, Jan. 2025.

[25] C. Camerer and T. H. Ho, "Experience-weighted attraction learning in normal form games," *Econometrica*, vol. 67, no. 4, pp. 827-874, Jul. 1999.

[26] B. Wang, C. Li, Y. Ban *et al*., "A two-tier bidding model considering a multi-stage offer-carbon joint incentive clearing mechanism for coupled electricity and carbon markets," *Applied Energy*, vol. 368, p. 123497, Aug. 2024.

[27] Z. Feng, L. Zou, and Y. Wei, "Carbon price volatility: evidence from EU ETS," *Applied Energy*, vol. 88, no. 3, pp. 590-598, Mar. 2011.

[28] R. Weron, "Electricity price forecasting: a review of the state-of-the-art with a look into the future," *International Journal of Forecasting*, vol. 30, no. 4, pp. 1030-1081, Oct. 2014.

[29] F. Li and R. Bo, "DCOPF-based LMP simulation: algorithm, comparison with ACOPF, and sensitivity," *IEEE Transactions on Power Systems*, vol. 22, no. 4, pp. 1475-1485, Nov. 2007.

[30] H.-P. Chao and R. Wilson, "Multi-dimensional procurement auctions for power reserves: robust incentive-compatible scoring and settlement rules," *Journal of Regulatory Economics*, vol. 22, no. 2, pp. 161-183, Sept. 2002.

[31] I. Energieagentur, *An Energy Sector Roadmap to Carbon Neutrality in China*. Paris: OECD Publishing, 2021.

[32] D. Newbery, "Missing money and missing markets: reliability, capacity auctions and interconnectors," *Energy Policy*, vol. 94, pp. 401-410, Jul. 2016.

[33] H. Eggleston, L. Buendia, K. Miwa *et al*. (2006, May). 2006 IPCC guidelines for national greenhouse gas inventories. [Online]. Available: https://www.ipcc.ch/report/2006-ipcc-guidelines-for-national-greenhouse-gas-inventories/

[34] P. Denholm, D. J. Arent, S. F. Baldwin *et al*., "The challenges of achieving a 100% renewable electricity system in the United States," *Joule*, vol. 5, no. 6, pp. 1331-1352, Jun. 2021.

[35] Ministry of Ecology and Environment of the People's Republic of China (2020). 2019 – 2020 implementation plan for national carbon emissions trading total allowance setting and allocation (power generation industry). [Online]. Available: https://www.mee.gov.cn/

[36] M. Rahimiyan and H. R. Mashhadi, "An adaptive Q-learning algorithm developed for agent-based computational modeling of electricity market," *IEEE Transactions on Systems, Man, and Cybernetics, Part C (Applications and Reviews)*, vol. 40, no. 5, pp. 547-556, Sept. 2010.

[37] Z. Yang, S. S. Raman, A. Shah *et al*., "Plug in the safety chip: enforcing constraints for LLM-driven robot agents," in *Proceedings of 2024 IEEE International Conference on Robotics and Automation*, Yokohama, Japan, May 2024, pp. 14435-14442.

[38] M. Mozikov, N. Severin, V. Bodishtianu *et al*., "EAI: emotional decision-making of LLMs in strategic games and ethical dilemmas," *Advances in Neural Information Processing Systems*, vol. 37, pp. 53969-54002, Dec. 2024.

[39] K. Hatalis, D. Christou, J. Myers *et al*., "Memory matters: the need to improve long-term memory in LLM-agents," *Proceedings of the AAAI*

Symposium Series, vol. 2, no. 1, pp. 277-280, Jan. 2024.
[40] L. Beurer-Kellner, M. Fischer, and M. Vechev, "Guiding LLMs the right way: fast, non-invasive constrained generation," in *Proceedings of the 41st International Conference on Machine Learning*, Vienna, Austria, Jul. 2024, pp. 3658-3673.
[41] X. Jiang, Y. Wu, C. Zhang *et al*., "DRoc: elevating large language models for complex vehicle routing via decomposed retrieval of constraints," in *Proceedings of the Thirteenth International Conference on Learning Representations*, Singapore, Apr. 2025, pp. 1-10.
[42] H. Trivedi, N. Balasubramanian, T. Khot *et al*., "Interleaving retrieval with chain-of-thought reasoning for knowledge-intensive multi-step questions," in *Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics*, Toronto, Canada, Jul. 2023, pp. 10014-10037.
[43] G. Marvin, N. Hellen, D. Jjingo *et al*., "Prompt engineering in large language models," in *Data Intelligence and Cognitive Informatics*. Singapore: Springer Nature, 2024, pp. 387-402.
[44] I. Gim, G. Chen, S.-S. Lee *et al*., "Prompt cache: modular attention reuse for low-latency inference," *Proceedings of Machine Learning and Systems*, vol. 6, pp. 325-338, May 2024.
[45] K. Acharya, W. Raza, C. Dourado *et al*., "Neurosymbolic reinforcement learning and planning: a survey," *IEEE Transactions on Artificial Intelligence*, vol. 5, no. 5, pp. 1939-1953, May 2024.

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