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Connecting the concepts of quantum state tomography and molecular representations for machine learning

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Quantum state tomography has been widely used to reconstruct the quantum state of a system from a set of informationally-complete measurements. Obtaining enough information about, *e.g.*, the wavefunction of a molecule allows its complete characterization. On the other hand, deep learning models have proven useful to perform molecular property prediction (forward design) and inverse design subject to property constraints within the approximate bounds of the data manifold, suggesting that their learned representations are reliable within the region of chemical compound space spanned by their training data. In this work, from the tomographic perspective, we argue that enforcing faithful prediction of an increasing number of diverse molecular descriptors from a shared learned representation progressively constrains the space of admissible internal explanations, driving the inter-alignment of models as they converge towards representation that can explain all observed properties. In the limit where the set of descriptors approaches information-completeness, this alignment drives the learned representations to states that can act, locally, as informationally-equivalent to the molecule's reduced quantum density matrix – a *deep tomography*. Under this lens, the generalization capabilities of a deep learning model, and the alignment among successful models, arise from unphysical or shortcut solutions becoming progressively incompatible as supervision approaches informational completeness.

1 Introduction

Information can be quantified through the outcomes of questions posed about a system.[1,2] Let $\mathcal{O}$ be a random variable taking values in a set of possible objects according to some probability distribution. Any question is a measurable function q whose outcome induces a conditional distribution over $\mathcal{O}$, leaving a remaining uncertainty quantified by $H(\mathcal{O}|q(\mathcal{O}))$, which satisfies $H(\mathcal{O}|q(\mathcal{O})) \leq H(\mathcal{O})$. Its answer may be discrete, in which case we can quantify its uncertainty using Shannon entropy, or continuous, in which case we use the differential entropy.[3] A set of questions $\mathcal{R} = \{q_l\}_{l=1}^{L}$ is sufficient for $\mathcal{O}$ if $H(\mathcal{O}|\mathcal{R}(\mathcal{O})) = 0$, meaning the answers completely determine $\mathcal{O}$, regardless of whether the set is overcomplete or contains redundant questions. Any such sufficient representation $\mathcal{R}(\mathcal{O})$ is a random variable satisfying

$$I(\mathcal{O};\mathcal{R}(\mathcal{O})) = H(\mathcal{O}), \tag{1}$$

where $H(\mathcal{O})$ quantifies the uncertainty of $\mathcal{O}$, and $I(\mathcal{O};\mathcal{R}(\mathcal{O}))$ is the mutual information between the object and its representation. In this way, $\mathcal{R}$ serves as the encoding of the object into a representation space.

In quantum chemistry, the main objects of interest are molecules, which are arrangements of interacting electrons and nuclei whose quantum mechanical state is described by a density matrix ρ. Such a density matrix contains all the information of the system.[4] It can be either a pure state (*e.g.*, the ground state), a Gibbs state representing a thermal state (*i.e.*, the equilibrium density operator of a system at temperature T for a given Hamiltonian), or any other state that quantifies the

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status of the molecule. Measuring observables on such quantum states can be thought of as asking a question about the molecule, and the resulting measurement outcomes as the answers to those questions.[5] Here, we refer to these answers as molecular descriptors, which contain information about structure, energy, electron density, spin state, oxidation state, or any other property of the system.

By measuring a sufficiently large set of properties of a molecule, known as an informationally-complete positive operator-valued measure (IC-POVM),[6–8] we can uniquely determine the density matrix *via* quantum tomography.[9–11] Because this set is informationally complete, any other molecular property can be reconstructed from it. We call the reconstruction from properties to properties a quantum property map (QPM)

$$f_{\mathrm{QPM}}\left(\mathcal{O} := \left\{\left\langle \hat{X}_l \right\rangle\right\}_{l=1}^{L}\right) = \left\langle \hat{Y} \right\rangle = \mathrm{Tr}\left(\rho \hat{Y}\right), \qquad (2)$$

where $\hat{X}_1$ and $\hat{Y}$ are quantum observables, and $\mathcal{O}$ is the set of properties that can be encoded in the molecule's density matrix ρ. Learning QPMs has been the target of deep learning models for molecular science, enabling molecular property prediction (forward design)[12–20] and inverse design subject to property constraints[21–23] within the bounds of the chemical space spanned by the training set, without explicit reference to the density matrix. In self-supervised learning, QPMs map inputs to an intermediate representation $\mathcal{R}(\mathcal{O})$ from which the original data can be recovered. Autoencoders $f_\theta = D_\theta \times E_\theta$ are the clearest example, with $\mathcal{R}$ produced by a learned encoder E_θ and inverted by a learned decoder D_θ. Here, each latent coordinate $(E_\theta(\mathcal{O}))_l$ is part of the model's information bottleneck[24–26] and can be interpreted as the answer to an unknown continuous-valued question about the input data $\mathcal{O}$. Training such a model is thus equivalent to learning an interrogation protocol that extracts the essential information of the object,[27] and determining the physical meaning of this interrogation process would enable meaningful AI explainability.[28–30] A QPM is learnable only when a well-defined input–output mapping exists. Otherwise, models can only resort to memorization (not interpolatable) or trivial statistical predictors (*e.g.*, mean regression under an MSE loss). For example, in a minimal quantum system such as a single spin-$\frac{1}{2}$ degree of freedom, a single descriptor given by $\langle S_z \rangle$ is insufficient to predict $\langle S_y \rangle$ since no functional map exists between them, in this case ML can only memorize training samples or perform trivial regression.

In a general setting, after successful training, these models learn structured representations that are semantically coherent: similar objects tend to map to nearby points in the learned representation space. This property enables interpolation and generative capabilities. Although a model must arrange objects in a semantically meaningful way in latent space to enable generative behavior,[31] there is no unique way to achieve this arrangement—because what counts as "semantic" is itself context-dependent. For example, benzene and pyridine are structurally very similar when viewed as molecular graphs, yet they differ greatly in their dipole moments. An even more striking case is thalidomide,[32] its two enantiomers are mirror images of each other, nearly identical structurally, yet their biological activities are drastically different.[33] Different contexts imply different semantic arrangements, and learning many competing contexts can force convergence towards representations that preserve physically meaningful information, assuming that the model is not exploiting spurious correlations as documented in the "Clever Hans" effect, where it was shown that some vision models had learned to correctly classify images by using the image's watermarks.[34,35]

Crucially, molecular descriptors are not independent labels: they are induced by a shared physical state. Here, we argue that if the data is obtained from informationally-complete observables, ML models learning QPMs converge towards an informationally-complete latent space that is semantically well-defined and behaves as a compressed representation of the system's quantum state, analogous to a state tomography reconstruction (*cf.* Fig. 1). Such models would effectively become surrogates for quantum mechanics, though likely in an approximate form, capturing only mean-field or low-order reduced density matrix information in the subset of the chemical space accessible through the dataset. We call this internal representation a *deep tomography* representation.

2 Information in one molecule

Molecules are composed of electrons and nuclei, which interact with each other through electromagnetic forces, and are represented by a wave function $|\Psi\rangle \in \mathcal{H}$ or density matrix $\rho \in \mathcal{H} \otimes \mathcal{H}^*$, where $\mathcal{H}$ is the system's Hilbert space. This defines the molecular Hamiltonian, the operator that dictates the energy, dynamics, and symmetries of the molecule:

$$\hat{H} = T_{\mathrm{n}} + T_{\mathrm{e}} + V_{\mathrm{nn}} + V_{\mathrm{ne}} + V_{\mathrm{ee}} \qquad (3)$$

where the Hamiltonian is decomposed into the kinetic energy of the nuclei (T_{n}) and electrons (T_{e}), together with the nucleus–nucleus (V_{nn}), nucleus-electron (V_{ne}) and electron–electron (V_{ee}) interaction potentials. In most cases, isolated molecules will relax to their ground state, which is the lowest eigenstate of $\hat{H}$ and molecules in a thermal bath will relax to a Gibbs state—a mixture of eigenstates of $\hat{H}$ weighted by their Boltzmann factor. In either case, finding the eigenstates of the molecular Hamiltonian helps us define what we mean by a molecule and, therefore, calculate its properties.

However, this many-body problem is intractable for large molecules since the dimension of the Hilbert space grows exponentially with the number of electrons and nuclei.[36,37] Even if we had a quantum computer that could store all the degrees of freedom of the full wave function of a molecule, solving for the ground or Gibbs state of a general molecule is a QMA-complete problem.[38–40] Thus, heuristic methods that make use of a compressed representation of the wavefunction, like Hartree–Fock,[41] DFT,[42] coupled cluster,[43] VQE,[44] or others, are needed and used to approximate the eigenstates.

When calculating molecular properties using these methods, it is common to express the Hamiltonian in second

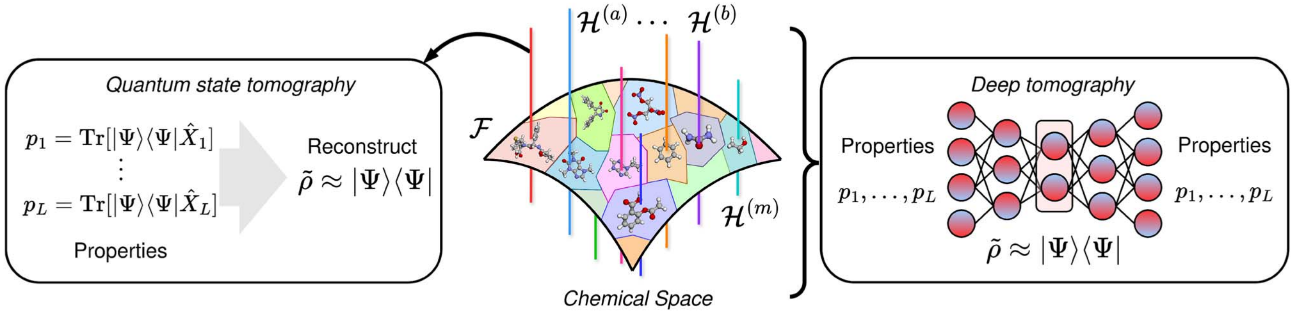

Fig. 1 Quantum state tomography is achieved by measuring a set of informationally-complete observables on a single molecule (left). Similarly, a *deep tomography* is a limit-behavior model that unifies an informationally-complete set of molecular descriptors in a shared representation object.

quantization, where operators are written in terms of creation and annihilation operators over a set of basis functions $\{\phi_\mu\}_{\mu=1}^{K}$ that span the relevant Hilbert space. In the standard Born–Oppenheimer approach, this basis is electronic only; however, the same formalism applies if the basis functions span the joint electron-nuclear space. On one hand, this formalism uses fewer degrees of freedom to approximate the molecular wave function compared to the first quantization representation. On the other hand, some properties, such as the fermionic and bosonic symmetries of the wave function, are easily encoded in the algebra of these creation and annihilation operators. The molecular Hamiltonian[36] can thus be written as

$$\hat{H} = \underbrace{\sum_{\mu,\nu} h_{\mu\nu} a_\mu^\dagger a_\nu}_{\text{one-body term: h}} + \underbrace{\frac{1}{2}\sum_{\mu,\nu,\lambda,\sigma} g_{\mu\nu}^{\lambda\sigma} a_\mu^\dagger a_\nu^\dagger a_\lambda a_\sigma}_{\text{two-body term: g}}, \tag{4}$$

where $h_{\mu\nu} = \langle\phi_\mu| - \frac{1}{2}\sum_i \nabla_i{}^2 |\phi_\nu\rangle$ are one-body integrals, $g_{\mu\nu}^{\lambda\sigma} = \langle\phi_\mu\phi_\nu|\sum_{i<j}\frac{1}{r_{ij}}|\phi_\lambda\phi_\sigma\rangle$ are two-body integrals, and $a_\mu^\dagger$ and a_μ are the creation and annihilation operator for the basis function ϕ_μ. Since $\hat{H}$ only depends on one- and two-body terms, calculating expectation values requires reduced information about the wave function, captured in the one- and two-body reduced density matrices.

Formally, a k-reduced density matrix (k-RDM) is a partial trace of the full density matrix $\rho = |\psi\rangle\langle\psi|$ over $N - k$ particles. The k-RDM is defined by

$$(\text{1st quantization}) \quad \Gamma^{(k)}\left(r_1, \ldots, r_k; r_1', \ldots, r_k'\right) = \binom{N}{k} \int \mathrm{d}r_{k+1} \ldots \mathrm{d}r_N \Psi(r_1, \ldots, r_N) \Psi^*\left(r_1', \ldots, r_k', r_{k+1}, \ldots, r_N\right),$$

$$(\text{2nd quantization}) \quad \Gamma^{(k)}_{i_1 \ldots i_k; j_1 \ldots j_k} = \langle\Psi|a_{i_1}^\dagger \cdots a_{i_k}^\dagger a_{j_k} \cdots a_{j_1}|\Psi\rangle,$$

and can be understood as a way of compressing the information of the complete wave function into fewer degrees of freedom—those corresponding to k particles. Some properties of interest, such as the electron density or the energy, can be expressed as a function of 1- or 2-RDM—as $\rho(r) = \mathrm{Tr}[\Gamma^{(1)}|r\rangle\langle r|]$ or $E = \mathrm{Tr}[\Gamma^{(1)}\mathrm{h}] + \frac{1}{2}\mathrm{Tr}[\Gamma^{(2)}\mathrm{g}]$. This raises the question: is the information in k-RDMs enough to reconstruct the full N-body wave function? This is the k-body N-representability problem.[45–49] Solving it for arbitrary k and N is NP-hard on classical computers[50] and QMA-hard for quantum computers,[49,51,52] but multiple heuristic methods are used to circumvent this issue.[53–55]

3 Information in many molecules

While the discussion so far has focused on a fixed quantum system with a defined number of particles, a foundation model that generalizes across chemistry must learn not only a representation of one system (as quantum tomography does), but also the shared representation across systems. This calls for a generalization of quantum tomography over Fock space, the space of quantum states across all molecular systems,[56,57] and the corresponding space of observables across molecules. Such a formulation may provide a natural framework for designing foundation models that aim to learn transferable QPMs across chemistry. By newly establishing a connection with quantum tomography, t hese ideas extend the formalization of chemical compound space (CCS) introduced by von Lilienfeld *et al.*.[58–60] The underlying complexity scales exponentially with Hilbert space dimension, although this challenge is partially mitigated by restricting attention to chemically relevant states.[61]

Fock space $\mathcal{F}$ is defined as the direct sum of Hilbert spaces over varying particle number $\mathcal{F} = \bigoplus_n \mathcal{H}^{(n)}$, where n enumerates "sectors" associated to a set of electrons and nuclei (*cf.* Fig. 1). Similarly, observables across molecules correspond to expectation values of operators acting on this Fock space. This unifying picture can guide architectural decisions in model design, helping ensure that learned representations respect physical principles already encoded in quantum theory. For instance, the indistinguishability of particles imply the foundation model should be permutationally invariant, and respect other symmetries depending on the systems being studied.

Another key aspect of this formulation is the notion of generalization across systems. All possible states of a molecule can be viewed as belonging to a sector. A foundation model should not only learn QPMs within single sectors (*cf.* eqn (2)), it should also be capable of learning the relationships between observables across different sectors,[58,62]

$$F_{\mathrm{QPM}}\left(\{\mathcal{O}_n\}_{n\in S}\right) \approx \left\langle \hat{Y} \right\rangle_{\mathcal{H}^{(m)}} = \mathrm{Tr}_{\mathcal{H}^{(m)}}\left(\rho^{(m)}\hat{Y}\right), \text{where } \mathcal{O}_n = \left\{\left\langle \hat{X}_l \right\rangle_{\mathcal{H}^{(n)}}\right\}_{l=1}^{L}, m \notin S. \tag{5}$$

Such cross-sector generalization is particularly relevant for frameworks that seek to infer properties of large systems by leveraging knowledge about smaller "motifs",[63–71] where the target quantum state in sector m, encoded in $\rho^{(m)}$, can be inferred from an informationally rich set of observables measured in other sectors, $\mathcal{X} := \{\mathcal{O}_n\}_{n\in S}$. This reflects the intuitive observation that motifs make similar contributions across different molecular systems,[72] while corrections emerge from the interactions among these substructures.[73] This is very well understood in quantum chemistry due to the locality of the coulomb operator, and for gapped systems the effects are restricted by such limits.[74,75]

Graph neural networks leverage this modular perspective by representing molecules as atomistic graphs, where message passing architectures learn to aggregate and propagate local information across systems.[12,76–79] Through iterative nonlinear transformations, these models aim to capture both local atomic environments and the aforementioned nonlocal correlations between molecular substructures. We formalize this idea with the *deep tomography* hypothesis discussed below.

4 The *deep tomography* hypothesis

Across vision, language, and materials, independently trained models on similar data tend to learn internal representations that are equivalent up to a simple transformation. This "alignment" has been observed empirically,[80–85] allowing, for instance, re-using layers from one network into another with minimal adaptation,[86,87] or translation between models' embedding spaces.[88,89] Different lines of work frame this in various ways: from practical tools like model stitching to more abstract proposals like the Platonic representation hypothesis,[90,91] its "strong" variant,[89] or the tomographic interpretation.[27] A recurring metaphor for this phenomenon is the Anna Karenina scenario: "all happy families are alike; each unhappy family is unhappy in its own way."[92] Well-generalizing models tend to converge on similar information-sufficient representations, while models that overfit, like "Clever Hans",[34] each fail in their own unique way. For a single descriptor, many distinct internal explanations, including unphysical shortcuts remain viable, as they can achieve low error on a single task.

The unifying insight across these perspectives is that well-trained models tend to arrive at one of a family of approximate information-sufficient representations.[25,93] This convergence arises from two complementary and interrelated mechanisms, which operate when supervision is mediated by a shared representation bottleneck: a common network trunk producing a single latent representation from which multiple targets are decoded. If targets are instead handled through separate disjoint networks the constraints do not accumulate on a common representation, and the convergence argument no longer applies. Moreover, the enforced targets must be sufficiently diverse: redundant or highly correlated descriptors do not impose additional constraints and thus do not meaningfully restrict the space of admissible representations.

4.1 Preservation of information

Integrating multiple views,[90,94–102] greatly constrains the solution space. Every property $\hat{X}_l$ encoded in the shared representation space restricts solutions $\theta^* \in \Theta_l$ to those minimizing the reconstruction error $d(\cdot,\ \cdot)$ for that property. Thus, in well-trained models every property $\hat{X}_l$ must be approximately recoverable (*cf.* eqn (6) and Fig. 2):

$$\boldsymbol{\Theta}* = \bigcap_{l=0}^{L} \boldsymbol{\Theta}_l, \boldsymbol{\Theta}_l = \left\{\theta*\middle|\operatorname{argmin}_\theta d\left(\mathcal{X}_l, \mathcal{Y}_l := D_\theta^l \circ E_\theta(\mathcal{X})\right)\right\} \tag{6}$$

4.2 Preservation of structure

In practice, the reconstruction error for $\hat{X}_l$ is minimized *via* a loss $\mathcal{L}$ (*e.g.*, mean squared error) over M molecular states:

$$\langle d(\mathcal{X}_l, \mathcal{Y}_l)\rangle \approx \frac{1}{M}\sum_{m=1}^{M}\mathcal{L}\left(p_l^m, q_l^m\right), \text{where } p_l^m \sim \mathcal{X}_l,\ \ q_l^m \sim \mathcal{Y}_l. \tag{7}$$

With limited data, an over-parameterized model can solve this by memorization (*i.e.*, a lookup table), failing to generalize effectively. However, given sufficient samples and model capacity, it must instead learn to minimize the reconstruction error across the full random variable $\hat{X}_l$, enabling interpolation. This is only possible if the representation $E_\theta(\mathcal{O})$ encodes information in a structured way, as discussed in the contrastive learning literature.[94,103–105] Specifically, for a valid similarity metric $\mathrm{Sim}_l(\cdot,\ \cdot)$, any ordering $\mathrm{Sim}_l(p_l^a,\ p_l^b) \leq \mathrm{Sim}_l(p_l^a,\ p_l^c)$ on realizations $p_l^m \sim \mathcal{X}_l$ must be preserved in latent space by a corresponding metric $\mathrm{Sim}_l'(\Gamma_{ML}^a, \Gamma_{ML}^b) \leq \mathrm{Sim}_l'(\Gamma_{ML}^a, \Gamma_{ML}^c)$ with $\Gamma_{\mathrm{ML}}^m \sim E_\theta(\mathcal{X})$.

When the model integrates another property $\hat{X}_{l+1}$, generalization demands that the latent space also preserve its similarity ordering Sim_{l+1}, which may conflict with that of $\hat{X}_l$. This structural encoding of potentially competing contexts imposes additional constraints, further narrowing the viable solution space.

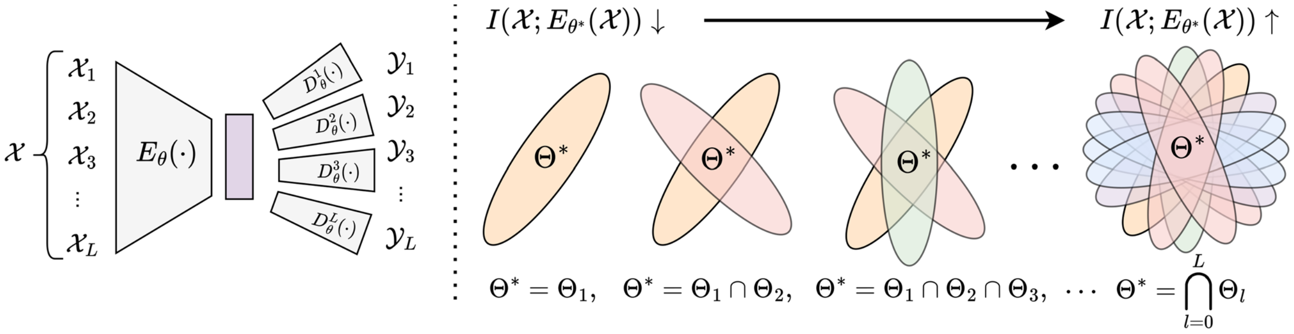

Fig. 2 Architecture for a QPM, where property l is reconstructed by a decoder D_θ^l from the latent space (left). Enforcing recoverability for multiple properties progressively increases the number of constraints on the solution space, driving convergence toward an informationally-complete subspace (right).

These constraints define an equivalence class of representations under invertible transformations that aim to approximately preserve both mutual information and local structure. The joint requirement to maintain semantic organization while satisfying multiple, potentially competing objectives sharply reduces the space of admissible solutions, providing a natural explanation for the convergence observed across independently trained models and sets the basis of transfer learning,[106–108] zero-shot learning[88] and the justification of foundation models.[101,109] According to the first postulate of Quantum Mechanics, the state of a physical system is completely described by its wavefunction. The k-RDM $\Gamma^{(k)}$ serves as the canonical object containing all k-body information about a quantum system.[110] We therefore propose the *Deep Tomography Hypothesis*: large ML models trained on molecular properties derived from the k-RDM will, in the limit of sufficient capacity and data, converge to latent representations that are informationally complete, and thus informationally equivalent to $\Gamma^{(k)}$ on the subset of the chemical space they are trained on. Importantly, even when an informationally-complete representation may not be accessible, *e.g.*, due to computational limits, or is not contained in a model's hypothesis space Θ, each model is biased towards the closest admissible approximation. Below, we formalize Hypothesis 1 and discuss its implications.

This hypothesis suggests that foundation models trained across many molecules and properties are, in effect, implementing a novel kind of cross-sector tomography. The model learns not only to interpolate within a sector of the Hilbert space, but also to extrapolate across different sectors of Fock space—a capacity that traditional quantum tomography does not possess, yet which is indispensable for scalable chemical prediction. Such models, when sufficiently expressive and trained on diverse molecular data, effectively extend the informational reach of quantum measurements: they enable predictions of quantum observables without direct quantum access to the system of interest, using knowledge transferred from related systems. This hypothesis should be understood as a statement on the limit behaviour, as in practice limitations regarding informational-completeness set of descriptors, model capacity and learning efficiency arise. In such non-ideal scenarios, the learned representations do not uniquely determine a sufficient statistics of the underlying quantum system consistent with all observed properties, but rather concentrate the probability mass over a subset of states consistent with the observations.

Hypothesis 1

Setup: let $\mathscr{X}$ be a dataset of L properties of M molecules $\mathscr{X} := \{\mathscr{O}_m = (p_1, p_2, \ldots, p_L)\}_{m=1}^{M}$, derived from a sufficiently rich set of observables on each molecule's k-RDM, $\Gamma^{(k)}$, approaching informational completeness. Let $F_\theta = D_\theta \circ E_\theta$ be a QPM defined by a sufficiently wide and expressive neural network, trained to predict these properties.
Hypothesis: the network's latent representation $\Gamma_{ML}^{(k)} := E_\theta(\mathscr{O}_m)$ of a molecule m tends toward an *informationally equivalent* encoding of $\Gamma^{(k)}$ for the subset of the chemical space accessible through $\mathscr{X}$. This is, if there exists a quantum operator $\hat{Y}$ such that $\mathrm{Tr}(\hat{Y}\Gamma^{(k)}) = p$, then, there exists a learnable decoder D_Y such that

$$\|D_Y(\Gamma_{\mathrm{ML}}^{(k)}) - p\| \leq \varepsilon,$$

with $\varepsilon \to 0$ in the data-capacity limit.

The conditions for the *deep tomography* hypothesis to hold rely on overcoming two bottlenecks: a data and a capacity bottleneck. The former assumes that we can reliably sample the massively large Fock space of chemicals. The latter assumes the model is sufficiently wide and deep. Since Hilbert spaces grow exponentially in the number of particles, a loose restriction on the underlying network is that it also be exponentially wide and deep. However, since these two limits are not feasible in practice, we believe the following:

- Width limit: since the dimension of the k-RDM is $O(N^{2k})$, *i.e.*, exponential in k and polynomial in the size of the underlying molecule, fixing a value for k will permit a reliable encoding of the k-RDM in a polynomial (in N) amount of neurons. The dimension of $\Gamma^{(k)}$ is the width of the model in this case, fixed for maximum size of the molecule considered.
- Depth limit: recovering the k-RDM from an informationally-complete set of properties is as expensive as a matrix inversion problem.[111] However, recovering $\rho = \Gamma^{(N)}$ from $\Gamma^{(k)}$ is QMA hard (*cf.* Section 2). This means that in the worst case, a network would need exponentially many layers to recover ρ but polynomially many layers to recover $\Gamma^{(k)}$.

This means that, for a fixed k, neither bottleneck is expected to be exponentially hard—making it feasible for the *deep tomography* hypothesis to be tested. We expect that this convergence in representation will be physically meaningful, allowing polynomially-large models to achieve transfer-learning capabilities.[112–114]

5 Outlook

The bitter lesson[115] has taught us that general ML models will get better as we scale compute and data.[116,117] In chemistry, larger and diverse datasets will give rise to the next generation of ML models, those capable of combining all types of information about molecules, crystals, proteins, materials, and other forms of matter—including structure, numerical properties, or other descriptors.[101] We believe these models will learn representations increasingly closer to informational-completeness, which we call deep tomographies, and these should be informationally equivalent to k-RDMs on the subset of the chemical space for which they are trained. Under this hypothesis, insights from quantum tomography, such as the role of information completeness, the structure of operator algebras, and the interpretability of reduced descriptions, can guide the design of better learning models. In particular, they motivate a move away from arbitrary descriptors toward physically grounded representations that preserve the relational structure among quantum observables.[112,118,119]

Viewed through this lens, symmetries and physical laws can be understood as additional physics constraints imposed on the model either through its architecture or the objective function. The difference lies not in the solution itself, which under the perspective adopted here would ultimately exhibit the required symmetries if enough and diverse data is provided, but in the optimization dynamics. While architectural enforcement of physics constraints can be beneficial in data-scarce regimes by ruling out unphysical solutions when those are viable,[120,121] such hard constraints may also restrict the optimization dynamics by disallowing temporary violations that could facilitate convergence toward a physically valid solution.[122,123] In data-rich regimes, this raises the question whether softer, penalty-based enforcement of constraints may allow more flexibility during optimization while leveraging the guidance they provide. Understanding this trade-off remains an open problem.

This work is conceptually related to PAC learning (Valiant's model),[124,125] while it addresses a different question. PAC learning assumes an unknown distribution $\mathcal{D}$ over a set of objects $\mathcal{O}$ and a target function $f : \mathcal{O} \to \{0, 1\}$. The central concern is whether access to labelled sample pairs $(o, f(o))$ drawn from $\mathcal{D}$, a learning algorithm can output a hypothesis $h \in \mathcal{H}$ that with high probability achieves small generalization error, with emphasis on sample and computationally efficiency. In contrast, we argue that in molecular science target functions are not arbitrary elements but induced by a shared physical variable, the molecule's quantum state. Enforcing faithful prediction over an increasing number of diverse molecular descriptors through a shared learned representation object, progressively restricts the space of admissible hypothesis. Unphysical or shortcut solutions become incompatible with all tasks, driving convergence toward representations that act like sufficient statistics, locally, of the underlying physics.

For quantum chemistry, this perspective hints at a path to foundation models that have tomographically-meaningful latent spaces, from which all other physical properties are recoverable. It suggests a principled and alternate benchmark procedure for representational completeness of foundation models beyond task-specific accuracy: freeze the encoder and train decoders to predict molecular properties not included during training. Models whose frozen representations support accurate reconstruction for a wider range of unseen observables can be regarded as more informationally-complete.

Such benchmarks can potentially bridge the gap between ML embeddings of molecules and quantum-mechanical state reconstructions—laying the groundwork for AI systems that operate as compressed yet faithful surrogates of the underlying physics. As the field advances, progress in foundation models for quantum chemistry coming from richer training data will enable the convergence towards deep tomographic representations. For example, the development of quantum computing will allow efficient computation of k-RDM properties of molecules[126–130] providing training data that surpasses the accuracy achievable by any classical simulation[131]—relevant for highly-correlated systems like FeMoco.[132] In such case, the ML architecture remains the same, but the dataset creation within a time-window is of higher quality. Another opportunity enabled by quantum processor would be access to learning algorithms with latent representations that are quantum in nature[26] and emerging devices like the 25–50 logical qubit machine "MAGNE"[133] would facilitate *deep tomography* representations learned from low-order measurements (1/2-RDMs) to serve as generalizable property-to-property maps, compressing complex many-body physics into experimentally grounded representations. In this second scenario, the ML model would be implemented as a quantum algorithm, and while we believe that the *deep tomography* hypothesis still hold—small changes on what is considered a decoder must be made. This would open a new practical route – or paradigm – to chemically reliable surrogates for strongly correlated motifs, supporting scalable prediction and validation of spin states, redox chemistry, and catalytic pathways in Fe–S type systems.[134] In summary, larger models trained on such data or algorithms, encompassing diverse molecular properties, will be better positioned to converge towards platonic representations capturing the essential structure of quantum-mechanical information.

Conflicts of interest

There are no conflicts of interest to declare.

Data availability

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