Challenges in sense-making and reasoning in the context of degenerate perturbation theory in quantum mechanics

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We discuss an investigation of student sense-making and reasoning in the context of degenerate perturbation theory (DPT) in quantum mechanics. We find that advanced undergraduate and graduate students in quantum physics courses often struggled with expert-like sense-making and reasoning to solve DPT problems. The sense-making and reasoning were particularly challenging for students as they tried to integrate physical and mathematical concepts to solve DPT problems. Their sense-making showed local coherence but lacked global consistency with different knowledge resources getting activated in different problem-solving tasks even if the same concepts were applicable. Depending upon the issues involved in the DPT problems, students were sometimes stuck in the "physics mode" or "math mode" and found it challenging to coordinate and integrate the physics and mathematics appropriately to solve quantum mechanics problems involving DPT. Their sense-making shows use of various reasoning primitives. It also shows that some advanced students struggled with self-monitoring and checking their answers to make sure they were consistent across different problems. Some also relied on memorized information, invoked authority and did not make appropriate connections between their DPT problem solutions and the outcomes of experiments. The advanced students in quantum mechanics often displayed analogous patterns of challenges in sense-making and reasoning as those that have been found in introductory physics. Student sense-making and reasoning show that these advanced students are still developing expertise in this novel quantum physics domain as they learn to integrate physical and mathematical concepts.

I. INTRODUCTION, FRAMEWORK AND GOAL

Sense-making is mapping or associating meaning to something in a given situation commensurate with the expertise of the individual or figuring out what is going on while solving a problem [1–8]. Unlike an exercise in which an individual is familiar with how to execute it, a problem is defined as a novel activity in which an individual must figure out how to achieve the goal in a fixed amount of time [9–14]. Thus, sense-making during physics problem-solving can be defined as the process that one goes through of figuring out what to do to solve a problem when they realize that there is a gap between what they already know and what the problem is asking for [1, 2]. One characteristic of expertise in a domain such as physics is that a well-organized knowledge structure of experts ensures that an expert's sense-making and reasoning are globally coherent and consistent [1–8, 15–19]. Expert-like sense-making also includes metacognitive tasks such as self-monitoring, regulation, and checking to ensure that the answers are reasonable [20]. Although expertise of different individuals can span a wide spectrum, the sense-making of students in physics courses who are developing expertise will only show local coherence and lack a global consistency [1, 2, 15].

Learning quantum mechanics (QM) is challenging even for advanced students partly due to the counter-intuitive nature of the formalism, which is very different from classical mechanics [21–24]. Prior studies suggest that many upper-level undergraduate and graduate students struggle while learning QM [23, 24] and research-based pedagogies and learning tools can help students learn quantum concepts better [25–29]. Many researchers have focused on developing conceptual surveys for evaluating student understanding of various quantum concepts [30–36] while others have investigated other aspects of learning QM, such as epistemological issues or student overconfidence [37, 38]. Also, to develop expertise in QM, students must develop a functional understanding of different representations commonly used in QM such as the Dirac notation [39–48]. Moreover, the second quantum revolution and its potential in transformative quantum technologies entail focus on workforce development [49–59]. This quantum information revolution has made it clear that we must help students develop a functional understanding of quantum physics in order to prepare them to play a role in developing, e.g., robust qubits and quantum gates to realize the potential of quantum technologies.

Some prior investigations have focused on helping students visualize quantum concepts [60–65] or learn QM via games [66] while others have investigated instructor and teaching assistants' attitudes regarding teaching QM including their grading approaches [67, 68]. Other researchers have focused on student difficulties after traditional lecture-based instruction including those related to quantum measurement [69–74], probability distributions for measuring physical observables, expectation values and their time dependence as well as student understanding of relative phase in the quantum states [43, 75–80], addition of angular momentum [81, 82], as well as with different quantum experiments [63, 83–91]. Other research studies have focused on cognitive issues, reasoning difficulties as well as transfer of learning specifically focusing on how they relate to the novel paradigm of QM [92–100]. Some researchers have focused on investigating student difficulties with other quantum concepts such as bound and scattering states, tunnelling and conductivity [101–103]. Other researchers have investigated student difficulties with finding a good basis for degenerate perturbation theory, fine structure corrections to the energy levels of the hydrogen atom, Zeeman effect, identical particles, total electronic energy of a free-electron gas, Fermi energy, and use of partial differential equation in QM [104–111]. Many researchers in the preceding work have also discussed development of research-based instructional materials and pedagogies to help students learn quantum concepts better.

Building on prior research studies that have focused on students' sense-making in the context of both classical and quantum mechanics problem solving [1–8, 15–18], here we focus on advanced students' sense-making after traditional lecture-based instruction in QM. If we want advanced students to become proficient in expert-like sense-making and reasoning in the context of quantum physics problem-solving, we must recognize that expert-like sense-making and reasoning involves integrating physical and mathematical concepts [1–8, 15–18] to build quantum mechanical models to explain phenomena that are observed or to predict those that have not been observed so far.

Prior research studies show that integrating physics and mathematics concepts coherently to solve physics problems is often challenging for students who are still developing expertise (e.g., see Refs. [1–8, 14, 15, 18, 112–115]). Mathematical sense-making in the context of solving physics problems can often be more difficult than when solving equivalent math problems without the physics context. Since working memory is constrained to a limited number of chunks and students' knowledge chunks pertaining to a concept are small when they are learning it, integrating physics and mathematics can increase the cognitive load during problem solving [116]. While sense-making, students often struggle to appropriately integrate the physical and mathematical concepts involved in solving a physics problem, and they sometimes make mathematical mistakes that they otherwise would not make if the physics context was absent [70].

Furthermore, we agree with Uhden et al. [3] on the difference between technical and structural roles of mathematics in physics and that "the technical skills are associated with pure mathematical manipulations whereas the structural skills are related to the capacity of employing mathematical knowledge for structuring physical situations". This view is consistent with Tzanakis's view [4] that "mathematics is the language of physics, not only as a tool for expressing, handling and developing logically physical concepts, methods and theories, but also as an indispensable, formative characteristic that shapes them, by deepening, sharpening, and extending their meaning, or even endowing them with meaning". Expert-like sense-making in solving QM problems using the quantum framework requires appropriate integration of both physical and mathematical concepts and the structural role of mathematics in the sense-making process is critical to solve QM problems. Therefore, an important aspect of expertise in QM is the proficiency with which one can integrate physical and mathematical concepts necessary to solve problems [3–7, 15–17]. In particular, developing expertise in quantum physics entails making appropriate math-physics connection to meaningfully unpack, interpret and apply the foundational tenets of quantum physics and use this sense-making during problem-solving to learn [3–8, 15–17, 19].

Marshman and Singh developed a framework [98] that emphasized how in both introductory physics and advanced QM, students come into their respective courses with diverse prior preparation, goals, and motivation and encounter a paradigm shift (everyday notions to classical physics or classical physics to QM). They demonstrated with examples that introductory students in classical mechanics and advanced students in QM display analogous patterns of difficulties while solving introductory or quantum physics problems (i.e., domains in which they are still developing expertise). Thus, since the paradigm of QM is very different from classical physics that advanced students are familiar with, it is important to recognize that meaningful sense-making to interpret and apply the quantum principles to solve problems, organize one's knowledge structure, and retrieve relevant knowledge to solve future QM problems using similar underlying principles can be challenging for even advanced students who may be proficient in classical physics.

The research presented here focuses on the analysis of the patterns of advanced students' sense-making and reasoning in the context of degenerate perturbation theory (DPT) as they try to make sense and integrate physical and mathematical concepts while solving problems in this novel QM paradigm. This investigation was conducted with students in upper-level undergraduate and graduate quantum mechanics courses. We find that advanced students often struggled to engage in expert-like sense-making consistent with the fact that they are still developing expertise in QM, and their knowledge structure in this area is only consistent locally so they are only looking for local coherence commensurate with their expertise while doing sense-making [117, 118]. Due to the fact that students' knowledge "chunks" are smaller than those of experts and working memory during problem-solving is limited [119], sense-making in the context of novel tasks in QM can become cognitively demanding and depending upon the contexts, different knowledge resources may get activated. This is particularly true for students who are struggling to develop expertise in QM due to the paradigm shift from classical to quantum mechanics [98].

The Knowledge in Pieces (KiP) framework by diSessa has been used to describe sense-making of students who are trying to develop expertise in a domain such as physics and how they use small, intuitive pieces of knowledge, which diSessa called "phenomenological primitives" or p-prims, to solve problems [117, 118]. Since students' knowledge structure is only locally coherent and lacks global coherence (their knowledge is in pieces), depending upon the specific features and context of a problem, different pieces of knowledge or “resources” may get activated [15]. For example, when trying to explain why it is warmer in the summer, novices may invoke the closer means stronger p-prim, which may be valid in other contexts, and claim that the earth must be closer to the sun in summer to explain the warmer temperatures. Another example is the larger means stronger p-prim that can lead novices to claim that in a collision between a large truck and a small car, the truck exerts a larger force on the car compared to the force the car exerts on the truck [117, 118]. In these types of responses, novices are using the larger is stronger p-prim as opposed to Newton’s Third Law, which states that the truck and car will experience the same magnitude force [117, 118].

Since these phenomenological primitives or p-prims [117, 118] are intuitive pieces of knowledge learned from everyday experience, there are a very large number of p-prims. In this study, instead of p-prims, we will focus on reasoning primitives following Tuminaro and Redish [15]. They [15] noted that “to reduce the extremely large number of p-prims and to group cognitive structures at their different levels of abstraction”, it may be useful to follow Redish’s [120] earlier work and “abstract from p-prims the notion of intuitive pieces of knowledge called reasoning primitives”. In the context of quantum mechanics in which the “intuitive” pieces of knowledge that students use as resources while solving problems are often not phenomenological (not derived from everyday phenomena) and we are not interested in very fine-grained resources at the level of p-prims, we focus on “reasoning primitives” [15]. Similar to p-prims, these reasoning primitives students use while solving problems, e.g., in the context of QM discussed here, lack global consistency although they show local coherence and lead to novice-like sense-making patterns. Also, here we use the phrases “reasoning primitives” or “reasoning heuristics” as mental shortcuts students use in different contexts even if it is possible to decompose them into finer-grained knowledge elements [15]. In particular, following Tuminaro and Redish [15], “the word “primitive” reflects the idea that these resources are “irreducible and undetectable” to the user—they are often used as if they were self-explanatory”. In this sense, reasoning primitives or reasoning heuristics discussed here are mental shortcuts that students use to solve QM problems even though the knowledge resources may be reducible into finer-grained knowledge elements. Also, as noted, in the context of QM, the distinction between intuitive and formal knowledge is blurry in that students’ intuitive knowledge resources do not necessarily have to be derived from things learned in everyday life experiences and could be from learning and recognizing certain patterns in other contexts. A facet of a reasoning primitive refers to its manifestation or instantiation in a particular situation. For example, in a study related to quantum computing [121], a facet of reasoning primitive “linear becomes exponential” (“linear in classical becomes exponential in quantum”) that was common in student responses is that a major difference between an N-bit classical and N-qubit quantum computer is that various things associated with number N for a classical computer should be replaced with number 2^N for a quantum computer (e.g., 2^N qubits must be initialized and 2^N bits of information are obtained as the output of the computation on the quantum computer).

Tuminaro and Redish [15] developed a framework after observing algebra-based introductory physics students’ sense-making while solving physics problems (that required integration of physics and mathematics) that accounts for the fact that students’ sense-making is only locally coherent. They also described common sense-making patterns in the students’ goal-oriented problem-solving tasks [15]. Tuminaro and Redish referred to these goal-oriented activities during problem solving as “epistemic games” and noted that an epistemic game can be defined as “a coherent activity that uses particular kinds of knowledge and processes associated with that knowledge to create knowledge or solve a problem” [15]. For example, some of the epistemic games students play include mapping meaning to mathematics, mapping mathematics to meaning, the physical mechanism game, and recursive plug-and-chug. In mapping meaning to mathematics “students begin from a conceptual understanding of the physical situation described in the problem statement, and then progress to a quantitative solution” [15]. When playing the mapping mathematics to meaning game, “students develop a conceptual story corresponding to a particular physics equation” [15] and then work through the corresponding mathematics to solve the problem. In the physical mechanism game, “students attempt to construct a physically coherent and descriptive story based on their intuitive sense of physical mechanism” [15] and then progress to a qualitative solution. When playing the recursive plug-and-chug game, students plug quantities into physics equations and churn out numeric answers, without conceptually understanding the physical implications of their calculations [15].

In this research, we take inspiration from these highly synergistic frameworks and discuss advanced students’ sense-making and reasoning while solving QM problems involving DPT and how they often used reasoning primitives. We find that similar to the p-prims in introductory physics, advanced students in quantum mechanics courses, who are still developing expertise, often use different reasoning primitives and the context often dictates which reasoning primitives are activated to solve a QM problem, e.g., related to DPT discussed here. Analogous to introductory physics students, advanced students’ sense-making during problem solving related to DPT using reasoning primitives displays coherence and consistency only locally, but typically does not possess the overall global consistency of an expert [15, 117, 118, 120]. We note that since our focus is not on symbolic forms [122], we will not discuss them here. Our findings show that advanced students struggle with sense-making and reasoning in the context investigated and in integrating concepts from QM and linear algebra to solve problems. We also find that without appropriate scaffolding support, advanced students solving QM problems may not display expert-like skills, e.g., they may not self-monitor, regulate, and check their answers to ensure that their problem solution is globally coherent. We classify advanced students’ challenges in sense-making and reasoning while solving QM problems involving DPT into four broad categories: (1) being stuck in the “physics mode” and using reasoning primitives based upon the physical context, (2) being stuck in the “math mode” and focusing on the mathematics involved in solving the problem but not accounting for the physical principles and concepts coherently, (3) inadequate self-monitoring, regulation, or checking of the answers to ensure global consistency, and (4) other epistemological issues. We illustrate each of these with specific cases involving advanced students' sense-making in different situations in the context of DPT.

Below, we present a qualitative analysis of the common challenges in advanced students' sense-making while solving DPT problems. Before discussing the patterns of students' sense-making and reasoning, we present the context in which this investigation was carried out: DPT involving the Zeeman effect (the hydrogen atom placed in an external magnetic field). We give examples of challenges in integrating physical and mathematical concepts in DPT, e.g., by analyzing the knowledge resources students activate when considering matrices relevant for different parts of the Hamiltonian and figuring out how to find a '*good*' basis for calculating the corrections to energies. Earlier we documented the development, validation and implementation of a tutorial on DPT involving the Zeeman effect [106, 107]. As noted, the focus here is on a qualitative analysis of advanced students' sense-making based upon different synergistic frameworks outlined in this section to highlight how different knowledge resources may get activated in different situations, how students may get stuck in the physics mode or math mode, and how they may struggle, e.g., to check whether their reasoning across contexts is consistent and use epistemological resources that are novice-like (e.g., reliance on memorized knowledge, invoking authority or not intentionally checking whether there is an appropriate connection between the inferences from their calculations and possible experimental outcomes). We also discuss how the sense-making and reasoning of advanced physics students in the context of quantum mechanics shares similarities to those exhibited by introductory students in introductory physics contexts.

Due to overlap in context, the following two sections (with background and methodology) have content taken directly from [104–107] for ease in understanding the content without looking at another paper. Also, the goal of this paper is to connect with a broader group of researchers who focus on sense-making regardless of the specific physics content of quantum mechanics unlike Ref. [106, 107]. Thus, even though the focus of this paper is on sense-making which is very different from our prior investigations, other sections in this paper may also have some overlap with Ref. [104–107] due to the context investigated.

II. CONTEXT FOR INVESTIGATING STUDENT SENSE-MAKING: DPT INVOLVING ZEEMAN EFFECT

A. Background For DPT

Perturbation theory is a useful approximation method for finding the energies and the energy eigenstates for a system for which the Time-Independent Schrödinger Equation (TISE) is not exactly solvable. The Hamiltonian $\hat{H}$ for the system can be expressed as the sum of two terms, the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation $\hat{H}'$, i.e., $\hat{H} = \hat{H}^0 + \hat{H}'$.The TISE for the unperturbed Hamiltonian, $\hat{H}^0\psi_n^0 = E_n^0\psi_n^0$, where ψ_n^0 is the n^{th} unperturbed energy eigenstate and E_n^0 is the n^{th} unperturbed energy, is exactly solvable. The energies can be approximated as $E_n = E_n^0 + E_n^1 + E_n^2 + \ldots$ where E_n^i for $i = 1, 2, 3..$ are the i^{th} order corrections to the n^{th} energy of the system. In non-degenerate perturbation theory (NDPT), the first-order correction to the n^{th} energy is

$$E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle \tag{1}$$

and the first-order correction to the n^{th} unperturbed energy eigenstate is

$$|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{(E_n^0 - E_m^0)}|\psi_m^0\rangle \tag{2}$$

in which $\{|\psi_n^0\rangle\}$ is a complete set of eigenstates of the unperturbed Hamiltonian $\hat{H}^0$. If the eigenvalue spectrum of $\hat{H}^0$ has degeneracy, the corrections to the energies and energy eigenstates are only valid provided one uses a *good* basis. For a given $\hat{H}^0$ and $\hat{H}'$, a *good* basis consists of a complete set of eigenstates of $\hat{H}^0$ that diagonalizes $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$ [123].

B. Background for DPT involving the Zeeman effect

For a hydrogen atom in an external magnetic field, one can use DPT to find the corrections to the energy spectrum [106, 107]. Using standard notation, the unperturbed Hamiltonian $\hat{H}^0$ of a hydrogen atom is $\hat{H}^0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$, which accounts only for the interaction of the electron with the nucleus via Coulomb attraction. The solution of the TISE for the hydrogen atom with Coulomb potential energy gives the unperturbed energies $E_n^0 = -\frac{13.6\text{eV}}{n^2}$, where $n = 1, 2, 3...$ is the principal quantum number. The perturbation is $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, in which $\hat{H}'_{fs}$ is the fine structure term and $\hat{H}'_Z$ is the Zeeman term [106, 107]. The Zeeman term accounts for the magnetic moments associated with the orbital and spin angular momenta in the external

TABLE I. Table of relevant operators, their eigenvalues, and a *good* basis for the hydrogen atom placed in an external magnetic field. All notations are standard.

Hamiltonian	Operator	Eigenvalues	*Good Basis*
Unperturbed Hamiltonian	$\hat{H}^0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$	$E_n = -\frac{13.6\text{eV}}{n^2}$	Both the coupled and uncoupled representation
Relativistic Correction	$\hat{H}'_r = -\frac{\hat{p}^4}{8m^3c^2}$	$-\frac{(E_n)^2}{2mc^2}\left[\frac{4n}{l+1/2} - 3\right]$	Both the coupled and uncoupled representation
Spin-Orbit Interaction	$\hat{H}'_{SO} = \frac{e^2}{8\pi\epsilon_0}\frac{1}{m^2c^2r^3}\vec{S}\cdot\vec{L}$	$\frac{(E_n)^2}{mc^2}\left\{\frac{n[j(j+1)-l(l+1)-3/4]}{l(l+1/2)(l+1)}\right\}$	Coupled Representation
Fine Structure	$\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$	$\frac{(E_n)^2}{2mc^2}\left(3 - \frac{4n}{j+1/2}\right)$	Coupled Representation
Zeeman Term	$\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$	$\mu_B B_{ext}(m_l + 2m_s)$	Uncoupled Representation

magnetic field. The Zeeman term is given by $\hat{H}'_Z = \frac{\mu_B B_{ext}}{\hbar}(\hat{L}_z + 2\hat{S}_z)$ in which $\vec{B}_{ext} = B_{ext}\hat{z}$ is a uniform, time-independent external magnetic field along the $\hat{z}$-direction, μ_B is the Bohr magneton and $\hat{L}_z$ and $\hat{S}_z$ are the operators corresponding to the z component of the orbital and spin angular momenta, respectively. The fine structure term includes a relativistic correction and the spin-orbit coupling term and is expressed as $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$. Here, $\hat{H}'_r = -\frac{\hat{p}^4}{8m^3c^2}$ is the relativistic correction term and $\hat{H}'_{SO} = \frac{e^2}{8\pi\epsilon_0}\frac{1}{m^2c^2r^3}\vec{S}\cdot\vec{L}$ is the spin-orbit interaction term (all notations are standard). Table I summarizes these terms.

We note that $\hat{H}^0$ for the hydrogen atom is diagonal when ANY complete set of orthogonal states is chosen for the angular part of the basis state (consisting of the product states of orbital and spin angular momenta). Thus, so long as the radial part of the basis state is always chosen to be a stationary state wavefunction R_{nl} for the hydrogen atom (for a given principal quantum number n and azimuthal quantum number l), the choice of a *good* basis amounts to choosing the angular part of the basis (the part of the basis that involves the product states of the orbital and spin angular momenta) appropriately. Therefore, we focus on the angular part of the basis to find a *good* basis and the corrections to the energies for the perturbation $\hat{H}'$ corresponding to the Zeeman effect in the hydrogen atom. For the angular part of the basis, states in the coupled representation $|l, j,\ m_j\rangle$ are labeled by the quantum numbers $l,\ s,\ j$, and m_j and the total angular momentum is defined as $\vec{J} = \vec{L} + \vec{S}$ (all notations are standard and $s = 1/2$ has been suppressed from the states $|l, j,\ m_j\rangle$ since $s = 1/2$ is a fixed value for a hydrogen atom). On the other hand, states in the uncoupled representation $|l,\ m_l,\ m_s\rangle$ are labeled by the quantum numbers $l,\ m_l$, and m_s (the notations are standard). Table I summarizes these results.

A basis consisting of states in the coupled representation forms a *good* basis for the fine structure term $\hat{H}'_{fs}$ and a basis consisting of states in the uncoupled representation forms a *good* basis for the Zeeman term $\hat{H}'_Z$, but not vice versa. Therefore, for the Zeeman effect, in which $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ and $\hat{H}'_{fs}$ and $\hat{H}'_Z$ are treated on equal footing (the corresponding energies are comparable with $E'_{fs} \approx E'_Z$), neither a basis consisting of states in the coupled representation nor a basis consisting of states in the uncoupled representation forms a *good* basis for the angular part to find perturbative corrections for the hydrogen atom placed in an external magnetic field. The following steps describe how to determine a *good* basis and find the first order corrections to the energy spectrum for the Zeeman effect: (1) choose a basis consisting of a complete set of eigenstates of $\hat{H}^0$ (e.g., one is free to choose a basis consisting of states in the coupled representation or a basis consisting of states in the uncoupled representation or any other basis), (2) write the $\hat{H}^0$ and $\hat{H}'$ matrices in the chosen basis, (3) identify $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$, (4) diagonalize the $\hat{H}'$ matrix in each degenerate subspace of $\hat{H}^0$ to determine a *good* basis, and (5) identify that the first-order corrections to the energy spectrum are the diagonal matrix elements of the $\hat{H}'$ matrix expressed as given by Eq. 1 in the *good* basis.

In the limiting cases of the strong and weak field Zeeman effects, the perturbation $\hat{H}'$ can be separated into two terms $\hat{H}' = \hat{H}'_{strong} + \hat{H}'_{weak}$, in which $\hat{H}'_{strong}$ is the stronger perturbation and $\hat{H}'_{weak}$ is the weaker perturbation. The corrections to the energies due to the stronger perturbation $\hat{H}'_{strong}$ are larger than the corrections due to the weaker perturbation $\hat{H}'_{weak}$. In these limiting cases, in order to find the corrections to the energies, one useful approach is to use DPT via a two-step approximation. In the first step, the stronger perturbation $\hat{H}'_{strong}$ is treated as the only perturbation. A good basis for step 1 is one that diagonalizes the unperturbed Hamiltonian $\hat{H}^0$ and also diagonalizes the stronger perturbation $\hat{H}'_{strong}$ in each degenerate subspace of the unperturbed Hamiltonian $\hat{H}^0$. After a good basis has been identified for step 1, the first order corrections for the stronger perturbation $\hat{H}'_{strong}$ are determined. In the second step of the two-step approximation, $\hat{H}^0_{strong} = \hat{H}^0 + \hat{H}'_{strong}$ is the new unperturbed Hamiltonian and the weaker perturbation $\hat{H}'_{weak}$ is treated as the perturbation. For step 2, a good basis is one that diagonalizes the unperturbed Hamiltonian $\hat{H}^0_{strong}$ and also diagonalizes $\hat{H}'_{weak}$ in each degenerate subspace of $\hat{H}^0_{strong}$. Once a good basis for step 2 has been identified, the first order corrections to the energies due to the weaker perturbation can be determined. The total first-order corrections to the energies are the sums of the corrections from steps 1 and 2.

The following steps describe how to determine a good basis and the first order corrections to the energies for the strong field Zeeman effect: (1) Treat the stronger perturbation $\hat{H}'_Z$ as the only perturbation on the unperturbed Hamiltonian $\hat{H}^0$, identify that a basis consisting of states in the uncoupled representation forms a good basis for the unperturbed Hamiltonian $\hat{H}^0$ and the stronger perturbation $\hat{H}'_Z$ (since $\hat{H}^0$ is diagonal in the uncoupled representation and $\hat{H}'_Z$ is diagonal in each degenerate subspace of $\hat{H}^0$ in the uncoupled representation), and determine the first-order corrections to the energies due to the stronger perturbation $\hat{H}'_Z$; (2) Treat the weaker perturbation $\hat{H}'_{fs}$ as the perturbation on $\hat{H}^0_Z = \hat{H}^0 + \hat{H}'_Z$, identify that a basis consisting of states in the uncoupled representation forms a good basis for the unperturbed Hamiltonian $\hat{H}^0_Z$ and the weaker perturbation $\hat{H}'_{fs}$ (since $\hat{H}^0_Z$ is diagonal in the uncoupled representation and $\hat{H}'_{fs}$ is diagonal in the degenerate subspaces of $\hat{H}^0_Z$ in the uncoupled representation), and determine the first-order corrections to the energies due to the weaker perturbation $\hat{H}'_{fs}$; (3) The sum of the first-order corrections obtained in steps 1 and 2 are the first-order corrections to the energy spectrum of the hydrogen atom. For the weak field Zeeman effect, the dominant fine structure term is the only perturbation on $\hat{H}^0$ in step 1 and the weaker perturbation $\hat{H}'_Z$ is the perturbation on the Hamiltonian $\hat{H}^0_{fs} = \hat{H}^0 + \hat{H}'_{fs}$ in step 2. In the weak field Zeeman effect, the coupled representation forms a good basis for both steps 1 and 2 [123].

III. METHODOLOGY

Students' sense-making and reasoning in QM in the context of DPT was investigated using both interview and written data. The presence of the interviewer was important to be able to discern that a given problem was novel for students and they were doing sense-making to solve the QM problem. On the other hand, written responses asking students to explain their reasoning were valuable to understand their reasoning (regardless of whether a given problem was novel for each student and required sense-making or whether students were simply articulating their reasoning for an exercise, i.e., a task they were familiar with from before because they had already seen that type of problem before and knew the solution). In particular, four years of data involving responses from 52 upper-level undergraduate students and 42 first-year graduate students to open-ended and multiple-choice questions administered after traditional lecture-based instruction in relevant concepts were analyzed. Students were asked to explain their reasoning. The undergraduates were in an upper-level (junior/senior level) undergraduate QM course, and graduate students were in a graduate-level core QM course. Insight about the student sense-making process was gained from 13 individual think-aloud interviews (a total of 45 hours) over the course of two years. Interviews were conducted with 3 undergraduate students who had completed two semesters of undergraduate QM and 10 graduate students who had completed two semesters of graduate level QM. We analysed sense-making while students reasoned during the individual interviews, which used a think-aloud protocol [124–126]. During the interviews, we did not disturb the students as they tried to solve the problems and only asked them for clarifications of points they had not made clear at the end. Written data were valuable for determining which aspects to probe further regarding student sense-making in the interviews. Students were provided with relevant information discussed in the background section and had lecture-based instruction in relevant concepts. Since sense-making patterns of undergraduate and graduate students involved in this investigation were similar, we do not separate their responses. We note that linear algebra is a prerequisite course for the upper-level undergraduate QM course.

The first two years of data from 32 undergraduates from clicker questions, quizzes, and exams were valuable for refining the questions further. Then we posed the following questions to 20 undergraduate and 42 graduate students as part of an in-class quiz after traditional instruction on DPT and to each of the 13 interviewed students. Some of the student reasoning patterns were inferred from these questions posed via written responses while most of the paper focuses on sense-making and reasoning uncovered during the interviews. Written data were valuable for determining which aspects to probe further regarding student sense-making in the interviews. We note that this paper only focuses on qualitative sense-making and reasoning.

To probe whether students were able to determine and do sense-making about the matrix elements of an operator that may be relevant for determining whether an angular basis (e.g., coupled representation, uncoupled representation, etc.) is *good* for the perturbations $\hat{H}'_Z$ and the spin-orbit interaction term $\hat{H}'_{SO}$ (which is part of the fine structure $\hat{H}'_{fs}$ along with the relativistic correction term $\hat{H}'_r$, i.e., $\hat{H}'_{fs} = \hat{H}'_{SO} + \hat{H}'_r$), the following are four examples of questions that were posed:

Q1(a). Evaluate the following matrix element useful for $\hat{H}'_Z$ for $n = 2$, in which the states are written in the coupled representation $|n,\ l,\ s,\ j,\ m_j\rangle$. **In order to receive credit, you must show your work or explain your reasoning.**

$$\left\langle 2,\ 1, \frac{1}{2},\ \frac{3}{2},\ \frac{3}{2}\right|(\hat{L}_z + 2\hat{S}_z)\left|2,\ 1, \frac{1}{2},\ \frac{3}{2},\ \frac{3}{2}\right\rangle$$

Q1(b-d). Evaluate the following matrix elements useful for $\hat{H}'_{SO}$ for $n = 2$, in which the states are written in the uncoupled representation $|n,\ l,\ s,\ m_l,\ m_s\rangle$. **In order to receive credit, you must show your work or explain your reasoning.**

(b) $\left\langle 2,\ 1,\ \frac{1}{2},\ 1, \frac{1}{2}\right| (\vec{S}\cdot\vec{L}) \left|2, 1,\ \frac{1}{2}, -1, \frac{1}{2}\right\rangle$

(c) $\left\langle 2,\ 1,\ \frac{1}{2},\ 1,\ \frac{1}{2}\right| (\vec{S}\cdot\vec{L}) \left|2, 1,\ \frac{1}{2}, 1, \frac{1}{2}\right\rangle$

(d) $\langle 2,\ 1,\ \frac{1}{2},\ 0,\ \frac{1}{2}|(\vec{S}\cdot\vec{L})|2,\ 1,\ \frac{1}{2},\ 1,\ -\frac{1}{2}\rangle$

Students were provided a table which contained relevant states in the coupled representation written in terms of linear combinations of states in the uncoupled representation. One method for answering Q1(a) is to write the state $|n,\ l,\ s,\ j,\ m_j\rangle = |2,\ 1,\ \frac{1}{2}, \frac{3}{2},\ \frac{3}{2}\rangle$ in the uncoupled representation as $|n,\ l,\ s,\ m_l,\ m_s\rangle = |2, 1,\ \frac{1}{2}\ 1,\ \frac{1}{2}\rangle$. Since the states in the uncoupled representation $|n,\ l, s,\ m_l,\ m_s\rangle$ are eigenstates of $\hat{L}_z$ and $\hat{S}_z$ with eigenvalues $m_l\hbar$ and $m_s\hbar$, respectively, the answer to Q1(a) is $[1+2(1/2)]\hbar = 2\hbar$.

Students were provided the equations $\vec{S}\cdot\vec{L} = \frac{1}{2}(\hat{J}^2-\hat{S}^2-\hat{L}^2) = \frac{1}{2}(\hat{L}_+\hat{S}_-+\hat{L}_-\hat{S}_+)+\hat{L}_z\hat{S}_z$ as well as the relevant eigenvalue equations and the equations for the raising and lowering operators $\hat{L}_\pm$ and $\hat{S}_\pm$ acting on states in the uncoupled representation that are helpful in answering Q1(b). Since $\hat{H}'_{SO}$ is proportional to $\vec{S}\cdot\vec{L}$, students must choose which equation is appropriate to calculate the matrix elements for a basis consisting of states in the uncoupled representation. For a basis consisting of states in the uncoupled representation, the equation $\vec{S}\cdot\vec{L} = \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z$ is more useful as states in the uncoupled representation are eigenstates of $\hat{L}_z$ and $\hat{S}_z$ and equations for the raising and lowering operators $\hat{L}_\pm$ and $\hat{S}_\pm$ acting on states in the uncoupled representation were provided to students. For Q1(b), after acting with the operator $\vec{S}\cdot\vec{L}$ on the ket state $|2, 1,\ \frac{1}{2}, -1, \frac{1}{2}\rangle$ in the uncoupled representation, the resulting states are orthogonal to the bra state $\langle 2,\ 1,\ \frac{1}{2},\ 1, \frac{1}{2}|$. Therefore, the answer to Q1(b) is zero. For Q1(c), $\langle 2,\ 1,\ \frac{1}{2},\ 1,\ \frac{1}{2}\big|\,(\vec{S}\cdot\vec{L})\,\big|2, 1,\ \frac{1}{2}, 1, \frac{1}{2}\rangle = \langle 2,\ 1,\ \frac{1}{2},\ 1,\ \frac{1}{2}\big|\,\hat{L}_z\hat{S}_z\,\big|2, 1,\ \frac{1}{2}, 1, \frac{1}{2}\rangle = \frac{\hbar^2}{2}$. For Q1(d), $\langle 2\ 1\ \frac{1}{2}\ 0\ \frac{1}{2}|(\vec{S}\cdot\vec{L})|2\ 1\ \frac{1}{2}\ 1\ -\frac{1}{2}\rangle = \langle 2\ 1\ \frac{1}{2}\ 0\ \frac{1}{2}|\hat{L}_-\hat{S}_+|2\ 1\ \frac{1}{2}\ 1\ -\frac{1}{2}\rangle = \frac{\sqrt{2}\hbar^2}{2}$.

In Q2, students' sense-making and reasoning were probed by asking them to identify the representations that make each of the operators $\hat{H} = \hat{H}^0$, $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_Z$ (that make up the different parts of the Hamiltonian for the Zeeman effect) diagonal in the degenerate subspace of $\hat{H}^0$.

Q2. *Circle* **ALL** *of the angular bases which make the Hamiltonian operator $\hat{H}$ diagonal in the $n = 2$ subspace of $\hat{H}^0$ and explain your reasoning. Assume that for all cases, the principal quantum number $n = 2$.*
i. Coupled representation,
ii. Uncoupled representation,
iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same l (i.e., states with different l values are not mixed),
iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same l (i.e., states with different l values are not mixed),
v. Neither coupled nor uncoupled representation.

In Q2, the operator $\hat{H}$ is a proxy for $\hat{H}^0$, $\hat{H}'_r$, $\hat{H}'_{SO}$, and $\hat{H}'_Z$ listed individually in four separate questions. Since $\hat{H}^0$ for a hydrogen atom is spherically symmetric with eigenvalues $E_n = -\frac{13.6eV}{n^2}$ and is diagonal when any complete set of orthogonal states with a fixed n is chosen for the angular basis, options i, ii, iii, and iv are all correct. The operator $\hat{H}'_r$ is also spherically symmetric with eigenvalues depending on n and l and is diagonal in the $n = 2$ degenerate subspace of $\hat{H}^0$ if the options i, ii, iii, or iv in Q2 are chosen as the angular basis. The operator $\hat{H}'_{SO}$ is diagonal in the $n = 2$ subspace if the angular basis consists of states in the coupled representation (option i only) in Q2. The operator $\hat{H}'_Z$ is diagonal if the angular basis consists of states in the uncoupled representation (option ii only) in Q2.

To probe student sense-making and reasoning regarding identifying a *good* basis for the given perturbation, the following is representative of a series of questions that were posed where $\hat{H} = \hat{H}^0 + \hat{H}'$. Students must build upon their reasoning for Q2 to now consider both the unperturbed Hamiltonian $\hat{H}_0$ and each of the listed perturbation $\hat{H}'$. A *good* basis depends on both $\hat{H}^0$ and $\hat{H}'$.

Q3. *A perturbation $\hat{H}'$ acts on a hydrogen atom with the unperturbed Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$. For the Hamiltonian $\hat{H}$, circle* **ALL** *of the representations that form the angular part of a good basis and explain your reasoning. Assume that for all cases the principal quantum number is fixed to $n = 2$.*
i. Coupled representation,
ii. Uncoupled representation,
iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same l (i.e., states with different l values are not mixed),
iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same l (i.e., states with different l values are not mixed),
v. Neither coupled nor uncoupled representation.

In the preceding question, the operator $\hat{H}'$ is a proxy for the operators $\hat{H}'_r$, $\hat{H}'_{SO}$, $\hat{H}'_{fs}$, $\hat{H}'_Z$, and $\hat{H}'_{fs} + \hat{H}'_Z$ that were listed individually in five separate questions.

In order to find the first-order corrections to the energies and energy eigenstates, one must first choose a *good* basis. Q2 focuses on the bases that form a *good* basis for the Zeeman effect with $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, as well as the individual operators $\hat{H}'_r$,

$\hat{H}'_{SO}$, $\hat{H}'_{fs} = \hat{H}'_r + \hat{H}'_{SO}$, $\hat{H}'_Z$. Knowledge of the bases that form a *good* basis for the individual operators $\hat{H}'_r$, $\hat{H}'_{SO}$, $\hat{H}'_{fs}$, $\hat{H}'_Z$ is helpful when reflecting upon a *good* basis for the Zeeman effect with the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$.

The unperturbed Hamiltonian $\hat{H}^0$ is spherically symmetric and therefore options i, ii, iii, and iv in Q3 all form a complete set of eigenstates of $\hat{H}^0$. Therefore, one must consider which set of basis states in Q3 also diagonalize the given $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$. Since the given degenerate subspace of $\hat{H}^0$ corresponds to $n = 2$, a *good* basis is one in which the perturbation matrix is also diagonal in that subspace. Considering each term of the perturbation separately, $\hat{H}'_r$ is diagonal if options i, ii, iii, or iv are chosen as the basis. Thus, a *good* basis for the perturbation due to the relativistic correction $\hat{H}'_r$ is given by each of the options i, ii, iii, and iv. The spin-orbit interaction term $\hat{H}'_{SO}$ is diagonal only for option i and thus only option i in Q3 forms a *good* basis for the spin-orbit interaction acting as the only perturbation. By a similar argument, option i in Q3 forms a *good* basis for the fine structure term as a perturbation. When the Zeeman term $\hat{H}'_Z$ acts as a perturbation on $\hat{H}^0$, only option ii forms a *good* basis.

The fine structure term $\hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}^0$ if the basis is chosen as states in the coupled representation (option i in Q3) and the Zeeman term is diagonal if the basis is chosen as states in the uncoupled representation (option ii in Q3), but not vice versa. Therefore, for the Zeeman effect, in which the perturbation is $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, neither a basis consisting of states in the coupled representation nor a basis consisting of states in the uncoupled representation forms a *good* basis so that option v in Q3 is the correct answer. In order to determine a *good* basis for the Zeeman effect, one may first choose a basis consisting of states in either the coupled or uncoupled representation and then diagonalize the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ in the degenerate $n = 2$ subspace of $\hat{H}^0$. This requires students to first be able to express either the $\hat{H}'_{fs}$ or $\hat{H}'_Z$ matrix in a basis that does not consist of a complete set of eigenstates in that subspace of that operator. For example, if a basis consists of a complete set of states in the coupled representation, then $\hat{H}'_Z$ is not diagonal and one must be able to express $\hat{H}'_Z$ in this basis (basis set does not consist of eigenstates of $\hat{H}'_Z$). Similarly, if a basis consists of a complete set of states in the uncoupled representation, then $\hat{H}'_{fs}$ is not diagonal and one must be able to express $\hat{H}'_{fs}$ in this basis.

We posed the following question to probe student sense-making and reasoning about the limiting cases of the strong and weak field Zeeman effects in the hydrogen atom (in which the limiting cases of the strong field and weak field Zeeman effects were listed individually in two separate questions):

Q4. *A perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ acts on a hydrogen atom with the unperturbed Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$. For the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$, circle* **ALL** *of the representations that form a good basis for the strong field Zeeman effect and explain your reasoning. Assume that for all cases the principal quantum number $n = 2$.*
i. Coupled representation,
ii. Uncoupled representation,
iii. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled representation with the same l (i.e., states with different l values are not mixed),
iv. Any arbitrary complete orthonormal basis constructed with linear combinations of states in the uncoupled representation with the same l (i.e., states with different l values are not mixed),
v. Neither coupled nor uncoupled representation.

The correct answer for the strong field Zeeman effect is option ii and the correct answer for the weak field Zeeman effect is option i for the reasons discussed earlier.

In an attempt to gain insight into students' sense-making and reasoning in determining whether an originally chosen basis was a *good* basis and then determining the first order corrections to the energies, we posed the following questions during the interviews. Since these questions involve a lower dimensional Hilbert space (compared to Q1-Q4 directly involving Zeeman effect), they provide additional insight into student sense-making in simpler contexts.

Q5. *Consider the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}'$, in which $\hat{H}^0 = V_0 \begin{pmatrix} 5 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ and $\hat{H}' = V_0 \begin{pmatrix} 0 & 0 & -4\epsilon \\ 0 & 2\epsilon & 0 \\ -4\epsilon & 0 & 2\epsilon \end{pmatrix}$ ($\epsilon << 1$ and $\hat{H}^0$ and $\hat{H}'$ do not commute), and the normalized basis states are $|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $|\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, and $|\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$. Determine the first order corrections to the energies.*

Here the originally chosen basis is a *good* basis and the first order corrections to the energies are 0, $2\epsilon V_0$, and $2\epsilon V_0$ (the diagonal matrix elements of $\hat{H}'$).

The next question was posed during the interviews to determine whether students would recognize that an originally chosen basis was not a *good* basis and their sense-making related to how to determine a *good* basis and the corresponding first order corrections to the energies.

Q6. *Consider the Hamiltonian* $\hat{H} = \hat{H}^0 + \hat{H}'$*, in which* $\hat{H}^0 = V_0 \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}$ *and* $\hat{H}' = V_0 \begin{pmatrix} 0 & \epsilon & \epsilon \\ \epsilon & 0 & \epsilon \\ \epsilon & \epsilon & 0 \end{pmatrix}$ *(*$\epsilon << 1$ *and* $\hat{H}^0$ *and* $\hat{H}'$ *do not commute), and the normalized basis states are* $|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $|\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ *, and* $|\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.
(a) Determine the first order corrections to the energies.
(b) Determine the first order corrections to the energy eignestates.

The originally chosen basis is a not *good* basis and one must first diagonalize the $\hat{H}'$ matrix in the degenerate subspace before determining the first order corrections to the energies.

Q7. *Consider the Hamiltonian* $\hat{H} = \hat{H}^0 + \hat{H}'$*, in which* $\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ *and* $\hat{H}' = V_0 \begin{pmatrix} -\epsilon & 0 & \epsilon \\ 0 & -\epsilon & 3\epsilon \\ \epsilon & 3\epsilon & \epsilon \end{pmatrix}$ *(*$\epsilon << 1$ *and* $\hat{H}^0$ *and* $\hat{H}'$ *do not commute), and the normalized basis states are* $|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $|\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ *, and* $|\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$*. Determine the first order corrections to the energies.*

The originally chosen basis is not a *good* basis and one must first diagonalize the $\hat{H}'$ matrix in the degenerate subspace before determining the first order corrections to the energies.

IV. CHALLENGES IN SENSE-MAKING AND REASONING

In order to develop expertise and be able to solve complex problems involving DPT, one must have a functional understanding of the relevant concepts in both QM and linear algebra, and be able to synergistically integrate and apply these physical and mathematical concepts as appropriate. In particular, in many problems, one must be able to move back and forth seamlessly between the physics and mathematics in the problem-solving process. It is imperative that as students do sense-making, they make these connections and apply the necessary concepts in each context while simultaneously reflecting upon the reasonability of their problem-solving process and solutions. Below, we discuss how advanced students sometimes used reasoning primitives and attempted to incorporate both the physics and mathematics but did so inconsistently. We also discuss how some advanced students did not engage in self-monitoring or checking their answers after solving a DPT problem. Finally, we discuss how other epistemological issues such as reliance on memorized knowledge, invoking authority, and inadequate consideration of the connection between the calculation and experimental outcomes may contribute to student challenges in sense-making and reasoning that requires integration of mathematical and physical concepts in the context of DPT. Table II summarizes the reasoning primitives used by the students related to DPT involving Zeeman effect but starts with one related to quantum computing [121] discussed earlier in the introduction section.

A. Physics Mode

We find that sometimes students made sense and reasoned about DPT problems primarily using reasoning primitives dependent upon the physical context or their physical intuition regarding the problem (i.e., they were in physics mode [18]). Oftentimes, the QM context may have suppressed activation of student knowledge resources related to correct linear algebra concepts in cases in which students would apply the same linear algebra concepts correctly if the QM context is not present. The use of reasoning primitives was sometimes based upon students' intuitive reasoning about one aspect of the physics of a problem and students sometimes did not explicitly write out all, or in some cases any, of the mathematical steps necessary to provide correct reasoning to solve a DPT problem. Below, we discuss some challenges students had with sense-making and reasoning as they focused primarily on the physics and did not appropriately account for the mathematics required to solve the problem.

1. Connecting the measurement of a physical observable to the corresponding concepts from linear algebra

Using the reasoning primitive facets that $\hat{H}\psi = E\psi$ is always true regardless of whether ψ is an energy eigenstate or that the Hamiltonian acting on a state corresponds to the measurement of energy: The TISE, $\hat{H}\psi = E\psi$, is an eigenvalue equation in which the Hamiltonian operator acting on an energy eigenstate ψ returns the same state multiplied by the energy eigenvalue. This equation is only satisfied when ψ is an energy eigenstate. One goal of DPT is to find approximate energy eigenvalues in situations in which the TISE $\hat{H}\psi = E\psi$ is not exactly solvable. An overemphasis on solving $\hat{H}\psi = E\psi$ for

TABLE II. Table of reasoning primitives and their facets. The first reasoning primitive "linear becomes exponential" is from a study involving basics of quantum computing [121] described in the introduction section. Although some reasoning primitive facets are broader (e.g., those related to TISE) than others, all other reasoning primitives are knowledge resources that students can activate in the context of solving DPT problems involving Zeeman effect.

Reasoning Primitive	Facets of the Reasoning Primitive
Linear becomes exponential	A major difference between an N-bit classical and N-qubit quantum computer [121] is that various things associated with number N for a classical computer should be replaced with number 2^N for a quantum computer (QC) e.g., 2^N qubits must be initialized and 2^N bits of information are obtained as the output of the computation on QC. Similarly, only N states are available for computation on an N bit classical computer etc.
Frequent means important	$\hat{H}\psi = E\psi$ rules all. $\hat{H}\psi = E\psi$ is the most fundamental equation of quantum mechanics and is true for all ψ.
Operator measures observable	In $\hat{H}\psi = E\psi$, the Hamiltonian operator $\hat{H}$ acting on a state ψ is equal to the energy E measured times ψ since $\hat{H}\psi$ corresponds to the measurement of energy.
Operator measures observable	$\hat{H}\psi = E$, the Hamiltonian operator $\hat{H}$ acting on a generic state ψ is equal to the energy E measured regardless of ψ since $\hat{H}\psi$ corresponds to the measurement of energy and collapses the state. (Prior investigations also show facets such as an operator corresponding to a physical observable acting on a state signifies measurement, e.g., $\hat{H}\psi = E_n\psi_n$ where the initial state ψ is not an energy eigenstate and ψ_n is an energy eigenstate in which the state collapsed after a measurement that yielded energy E_n [34, 69, 70, 127].)
Convenient means mandatory	Convenient bases are the only possible bases for a given physics problem.
Some parts rule	A *good* basis in DPT only depends on the unperturbed Hamiltonian $\hat{H}^0$ (no dependence on perturbation Hamiltonian).
Some parts rule	A *good* basis in DPT only depends on the perturbation Hamiltonian $\hat{H}'$ (no dependence on unperturbed Hamiltonian).
Everything matters	One must diagonalize the entire $\hat{H}'$ matrix instead of just a subspace in which $\hat{H}^0$ has degeneracy to find good basis.
Part represents whole	A *good* basis for one of the terms in the perturbation must be a *good* basis for the entire perturbation.
Combining things maintains features	Superposition maintains eigenstate. A linear combination of energy eigenstates MUST be an energy eigenstate.
Combining things destroys features	Superposition destroys eigenstate. A linear combination of energy eigenstates can NEVER be an energy eigenstate.

various $\hat{H}$ (not only in the context of perturbation theory but in general in QM courses) leads students to use the reasoning primitive "frequent means important" while contemplating about $\hat{H}\psi = E\psi$. For example, some students thought that this equation is the most fundamental equation of QM and is true regardless of whether ψ is an energy eigenstate consistent with prior findngs [69]. Table II shows that another reasoning primitive is "operator measures observable". A facet of this reasoning primitive reported previously is that an operator corresponding to a physical observable, e.g., Hamiltonian, acting on the state of a quantum system signifies a measurement of the corresponding observable, e.g., energy [34, 69, 70, 127]. Some interviewed students correctly stated that the result of a measurement returns a value of the observable measured. However, they incorrectly added that in $\hat{H}\psi = E\psi$, the Hamiltonian operator $\hat{H}$ acting on a state ψ is equal to the energy E measured times ψ since $\hat{H}\psi$ corresponds to the measurement of energy. Other students used a different facet of the same reasoning primitive to conclude that the Hamiltonian operator $\hat{H}$ acting on the state ψ gives the energy measured regardless of the state and would yield $\hat{H}\psi = E$. They omitted the state from the right-hand side of the TISE. Also, $\hat{H}\psi = E$ is dimensionally inconsistent. However, these students' sense-making did not involve activation of relevant linear algebra resources pointing to this inconsistency. For example, they did not draw from their linear algebra background to realize that an operator acting on a vector cannot possibly return simply the energy which is a scalar (instead, it must return a vector quantity). Students with this type of sense-making were in the physics mode and often struggled in connecting the physics and mathematics appropriately. Prior investigations show other facets of this reasoning primitive (operator measures observable), e.g., $\hat{H}\psi = E_n\psi_n$, where the initial state ψ is not an energy eigenstate and

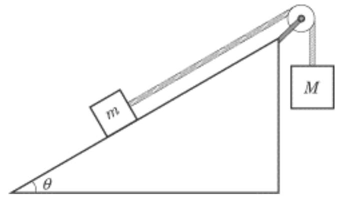

FIG. 1. A common system encountered in introductory physics in which some students think that there are only two possible choices of coordinate axes (horizontal-vertical and parallel-perpendicular to the inclined plane).

ψ_n is an energy eigenstate in which the state collapsed after the measurement that yielded energy E_n [34, 69, 70, 127].

2. Challenges in connecting concepts involved for choosing a basis in QM with similar concepts in linear algebra

Reasoning primitive "convenient means mandatory" manifests as convenient bases are the only possible bases for a given problem: Oftentimes students were so focused on the coupled and uncoupled representations for a basis and when each would be a convenient choice for a given operator, that they did not activate resources related to the fact that there are other choices for the basis in a given problem. When asked to determine bases in which an operator is diagonal in Q2 and the *good* bases in Q3, some interviewed students struggled to unpack the meaning of "any arbitrary complete orthonormal basis constructed with linear combinations of states in the coupled/uncoupled representation" (options iii/iv). One student stated "I thought there was only the coupled and uncoupled representation. What would a linear combination of the coupled states be?" While the coupled and uncoupled representations are often the most convenient choices for the angular part of the basis, they are not the only choices. Students with this type of sense-making challenge did not activate resources pertaining to the fact that while the coupled and uncoupled representations are often convenient choices for the angular basis, these are merely two arbitrary bases. These students also did not reflect upon the fact that if the initial angular basis is not a *good* basis when either the coupled or uncoupled representation is chosen, then a *good* basis must be constructed from a linear combination of the states in the coupled (or uncoupled) representation. For example, this is the case for the intermediate field Zeeman effect, in which the perturbation is $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$.

This type of sense-making challenge arises when applying linear algebra in the context of quantum mechanics and is analogous to sense-making challenges introductory students face with the choice of basis in introductory physics [128]. For example, thinking that there are only coupled and uncoupled bases in QM is analogous in the context of introductory physics to incorrectly thinking that there is only one choice for the coordinate system (the basis that is used most conventionally) or that there are only two possible coordinate systems, e.g., for a block on an inclined plane with a certain angle such as that in Figure 1. Some introductory students think that choosing a basis in which the basis vectors are parallel and perpendicular to the inclined plane or basis vectors that are horizontal and vertical are the only possible choices. In particular, in these cases, students may struggle with the fact that these basis vectors may be the most convenient, but nothing prohibits one from choosing any other set of two independent vectors as the basis vectors. In the study conducted by Volkwyn et al. [128], when researchers found that introductory students may view Cartesian coordinate systems as being fixed in standard orientations, they provided students with opportunities to notice the movability of coordinate systems in a lab designed for it. Even in a two-dimensional space, there are infinitely many possible bases consisting of two linearly independent vectors. One must apply analogous reasoning in the context of the QM problem posed in Q3 when considering the possible angular bases but this type of sense-making was challenging for these advanced students. We note that if students were only asked about the number of possible bases one can choose for a two dimensional vector space, they may answer the question correctly but the physics context makes them focus only on the convenient bases in those problems.

3. Focusing on only one aspect of a system rather than the entire system

Students were generally able to make the connection that the energy values they were solving for are the eigenvalues of the Hamiltonian operator. Often times students would relate the diagonal matrix elements of the Hamiltonian operator expressed in matrix form to energy values. However, they would focus primarily on $\hat{H}^0$ or $\hat{H}'$ for determining a good basis for finding the energies.

In DPT, the energies are approximated as the sum of the unperturbed energies (which can be determined exactly from the unperturbed Hamiltonian $\hat{H}^0$) and the perturbative corrections to the energies (determined from the perturbation $\hat{H}'$). Therefore, one must consider both $\hat{H}^0$ and $\hat{H}'$ when determining a *good* basis and the corrections to the energies. If one only focuses on the

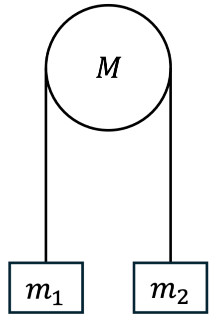

FIG. 2. A common system encountered in introductory physics involving two masses suspended from a pulley with mass.

perturbation $\hat{H}'$, then one neglects the contribution due to the dominant term in the energy from the unperturbed Hamiltonian. If instead, one only focuses on the unperturbed Hamiltonian $\hat{H}^0$, then one loses the point of DPT, which is to find the corrections to the unperturbed Hamiltonian due to the perturbation $\hat{H}'$. We find instances of student sense-making in which they considered only $\hat{H}^0$ or $\hat{H}'$, but not both when determining a *good* basis and finding the first order corrections to the energies. Additionally, students' sense-making showed how challenging it is to consider the consequences of diagonalizing the perturbation matrix $\hat{H}'$ (either the entire $\hat{H}'$ matrix or $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$) and how this affects $\hat{H}^0$.

This type of struggle in sense-making, in which one has a system comprised of a number of different components that must be considered and combined coherently, is common in different areas of physics [129]. For example, in introductory physics, students often consider a system with pulleys and masses (an example is shown in Fig. 2). If the pulley has a mass, students struggle even more in sense-making than if the pulley did not have a mass [130–134]. To solve for the unknowns in Fig. 2, one must consider the forces acting on each of the suspended masses and the net torque acting on the pulley [131–134]. One sense-making pattern is for students to start with only the consideration of the forces acting on the two suspended masses and to ignore the mass of the pulley and the corresponding torque.

Below we discuss examples of students focusing only on one part of the Hamiltonian rather than both the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation $\hat{H}'$. We note that we include these examples in the physics mode section since some students' sense-making shows that they only focused on unperturbed Hamiltonian or perturbation Hamiltonian for finding a good basis at least partly because they thought that those parts are the only relevant parts for finding a good basis based upon the physics involved.

Reasoning primitive "some parts rule" manifests as a *good* basis only depends on $\hat{H}^0$: Some students chose a *good* basis based upon the representation that makes $\hat{H}^0$ diagonal without considering whether the operator $\hat{H}'$ is diagonal in that basis. For example, on question Q2, some students incorrectly selected only the uncoupled representation (option ii) as the basis that would make the operator $\hat{H}^0$ diagonal and they then incorrectly chose the uncoupled representation as a *good* basis for $\hat{H}^0$ and $\hat{H}'_{SO}$ in Q3. In their explanation, they noted that states in the uncoupled representation were eigenstates of $\hat{H}^0$, but they did not consider the fact that $\hat{H}'_{SO}$ is not diagonal in each degenerate subspace of $\hat{H}^0$ when states in the uncoupled representation are chosen as the basis states.

In the interview, students with this type of sense-making pattern often focused on the bases that make $\hat{H}^0$ diagonal (thinking that part was the only relevant consideration) but did not consider the fact that the perturbative corrections obtained in DPT depend on the perturbation $\hat{H}'$. Using this type of reasoning, one would obtain the same *good* basis for $\hat{H}^0 + \hat{H}'$ regardless of the perturbation $\hat{H}'$ in a given situation. Furthermore, the perturbative corrections one obtains from an initial basis consisting of a complete set of unperturbed energy eigenstates will provide meaningless corrections unless one ensures that the basis also diagonalizes $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$.

Reasoning primitive "some parts rule" manifests as a *good* basis only depends on $\hat{H}'$: Other students chose a *good* basis based upon the representations that make $\hat{H}'$ diagonal without considering whether the operator $\hat{H}^0$ is diagonal in that basis. For example, in response to Q2, some students incorrectly selected only the uncoupled representation (option ii) as the basis that would make $\hat{H}^0$ diagonal and also incorrectly selected the coupled representation (option i) in Q2 as the only basis that would make $\hat{H}'_r$ diagonal in the degenerate subspace of $\hat{H}^0$. These students then incorrectly chose the coupled representation as the only *good* basis for $\hat{H}^0$ and $\hat{H}'_r$ in Q3. While these students were correct that states in the coupled representation form a *good* basis, they used incorrect reasoning to formulate their answer and also did not identify that all the options i, ii, iii, and iv are correct for $\hat{H}'_r$ in Q3.

In the interview, students with this type of response had sense-making patterns that often focused on Eqs. 1 and 2 and only considered the matrix elements of $\hat{H}'$ when determining the first order perturbative corrections. They neglected the fact that unperturbed energies are the dominant terms and that one must always ensure that the basis is a complete set of unperturbed energy eigenstates.

Some students' sense-making patterns showed that they did not activate resources related to the fact that when the originally chosen basis is not already a *good* basis and the unperturbed Hamiltonian $\hat{H}^0$ and the perturbing Hamiltonian $\hat{H}'$ do not commute, they must diagonalize the $\hat{H}'$ matrix only in each degenerate subspace of $\hat{H}^0$.

Interviews suggest that some students struggled with the fact that if $\hat{H}^0$ and $\hat{H}'$ do not commute, diagonalizing $\hat{H}'$ produces a basis in which $\hat{H}^0$ is not diagonal. Since $\hat{H}^0$ is the dominant term and $\hat{H}'$ provides only small corrections, we must ensure that the basis states used to determine the perturbative corrections in Eqs. 1 and 2 remain eigenstates of $\hat{H}^0$.

Additionally, some students' sense-making patterns show that they only focused on $\hat{H}'$ and did not consider whether the originally chosen basis was already a *good* basis. For example, students were given question Q5. In this case, $\hat{H}'$ is already diagonal in each degenerate subspace of $\hat{H}^0$ and the first order corrections to the energy are the diagonal matrix elements of $\hat{H}'$ so no additional calculations are necessary. However, students who only focused on $\hat{H}'$ thinking that was the only relevant part for finding the corrections to the energies often proceeded to diagonalize the entire $\hat{H}'$ matrix.

In the interview, when asked to determine the first order corrections to the energies, some students recalled a previous example in which the energy spectrum of $\hat{H}^0$ in the current problem had the same degenerate energy values as the previous problem. In that case, it is valid to diagonalize the entire $\hat{H}'$ matrix as the degenerate subspace of $\hat{H}^0$ is the entire matrix. However, students overgeneralized this approach and applied it to each DPT problem. Interviews suggest that they oftentimes began diagonalizing the entire $\hat{H}'$ matrix without even considering the degeneracy of the energy spectrum of $\hat{H}^0$ and the commutation relation between $\hat{H}^0$ and $\hat{H}'$. If $\hat{H}^0$ and $\hat{H}'$ do not commute, then the basis found by diagonalizing the $\hat{H}'$ matrix is no longer a complete set of eigenstates of $\hat{H}^0$ and cannot possibly be a *good* basis.

B. Math mode

As is common when students are developing expertise in physics, they may focus on the mathematics but not necessarily integrate it appropriately with physical principles when solving a problem (i.e., they are in the math mode [18]). In the context of DPT, student sense-making suggests that oftentimes they started with equations that appear to have the appropriate variables and began manipulating the equations and plugging in numbers without analyzing the problem to ensure that the formulas are appropriate and match the physical situation. In some situations, some students followed a recursive "plug and chug" approach [15] until they reached an answer that appeared to answer the question posed in the problem to their satisfaction without giving any consideration to the physical context or checking to make sure that their answer is reasonable.

1. Recursive plug-and-chug in applying the raising and lowering operators

The operator $\hat{H}'_{SO}$ can be expressed in terms of the raising and lowering operators $\hat{L}_\pm$ and $\hat{S}_\pm$. While the raising and lowering operators are not Hermitian and do not correspond to physical observables, they can be combined to determine the contribution to the Hamiltonian due to the spin-orbit interaction term. The utility of the raising and lowering operators is that they provide an efficient way to describe what an operator acting on a given state in the uncoupled representation would yield. For example, for an electron in the hydrogen atom, the raising operator $\hat{S}_+$ acting on a state with quantum number m_s increases the quantum number by one to $m_s + 1$. Since the quantum number m_s is restricted to values between $-s$ and s, the raising operator acting on a state with $m_s = s$ must return zero times the new state as this state is not physically possible. Similarly, it is not possible to "lower" a state with $m_s = -s$. The expressions for the raising and lowering operators will produce a coefficient of zero for these physically impossible situations. However, in interviews, we find that students occasionally made an algebraic mistake when evaluating matrix elements in Q1(b) when determining these coefficients and as a result generated a quantum state that is physically impossible. However, their sense-making during the problem-solving process did not involve time to reflect and check whether their final answer corresponded to a physically consistent answer.

In particular, these students' sense-making did not involve reasonability check or connecting the physical situation to the problem at hand. They were so focused on the equations and performing the calculations that they did not reflect upon the physical situation prior to starting the problem and after arriving at an answer that was inconsistent with the given situation. On the other hand, if a physics expert were given a problem that involved dealing with evaluating the raising operator $\hat{L}_+$ acting on a state with quantum number $m_l = l$, then the expert would use qualitative reasoning to determine that the expression must be 0 without an explicit calculation. Additionally, experts would also reflect upon their final answer and realize that there is an inconsistency in their calculation if they obtained a final answer including a quantum state that is not physically possible. However, since these students are still developing expertise in QM, their sense-making often shows that it is challenging for them to use qualitative reasoning consistently and correctly to solve a problem. Due to limited cognitive resources while problem-solving involving these QM problems, these types of challenges may sometimes be due to inability to access appropriate cognitive resources while sense-making to perform checks and ensure that their final answers are reasonable.

2. *Focusing on equations for the first order corrections without connecting to the physical model*

When solving DPT problems, some students engaged in the mapping mathematics to meaning epistemic game. They began with an equation and worked through the mathematics only to consider the physical context when it came time to report the final answer. These students started the problem with a mathematical model and then tried to connect it to the physical model and physical phenomenon, but did not engage in expert-like sense-making to ensure that their mathematical model was correct and globally coherent. While knowing when to use which equation is of paramount importance in solving any physics problem, we find that some advanced students struggled with using the correct equations in the context of DPT. Below, we discuss student sense-making and reasoning challenges when they pursued a problem-solving approach in which they began applying and manipulating equations before spending adequate time considering the physical context and planning the problem solution conceptually.

Incorrectly categorizing the problem as a non-degenerate perturbation theory (NDPT) problem: The unperturbed energies for the hydrogen atom only depend on the principle quantum number n. As noted, for each value of n, there are $2n^2$ degenerate states corresponding to all the possible values of l, m_l and m_s (due to the spin degrees of freedom). Therefore, in order to find the perturbative fine structure corrections to the energy of the hydrogen atom, one must use DPT. However, some students did not activate resources related to the fact that they had to use DPT, and instead used the equations from non-degenerate perturbation theory to find the first-order perturbative corrections to the energies. These students did not consider the degeneracy in the energy spectrum of the unperturbed Hamiltonian $\hat{H}^0$ in order to ensure that using Eqs. 1 and 2 is valid for the problem.

Interviews suggest that students with this type of sense-making were often focusing on the equations for the first order corrections without reflecting upon the physical situation carefully. They did not take into account that if there is a degeneracy in the energy spectrum of $\hat{H}^0$, then one must first determine a *good* basis before determining the perturbative corrections; otherwise the expressions in Eqs. 1 and 2 are not valid.

Using DPT to find corrections to the wavefunctions but not using DPT to find the first-order corrections to the energies: Students with this type of sense-making appeared to be using reasoning that was locally consistent but not globally consistent. They did not take into account the fact that a *good* basis for finding corrections to the energy eigenstates must also be a *good* basis for finding corrections to the energies. For question Q6(b), most of the interviewed students activated knowledge resources that the first order corrections to the energy eigenstates $|\psi_n^1\rangle$ are not valid unless we choose a *good* basis. When examining Eq. 2, they identified that there will be terms in which the denominator is zero due to the degeneracy in the energy spectrum. However, some of these same students thought that Eq. 1 is still valid to find the first order corrections to the energies since no divergent terms appear in Eq. 1. They claimed that any basis which consists of eigenstates of $\hat{H}^0$ is a *good* basis for finding the first order corrections to the energies, but that this same basis may not be a *good* basis for finding the first order corrections to the energy eigenstates. They did not realize that in order to find any perturbative corrections (to the energies or energy eigenstates), the basis is a *good* basis only if $\hat{H}'$ is diagonal in each degenerate subspace of $\hat{H}^0$ in addition to $\hat{H}^0$ being diagonal. If a basis is not a *good* basis for finding the corrections to the energy eigenstates, then that same basis cannot be a *good* basis for finding the corrections to the energies. When calculating the first order corrections to the energies, students with this type of sense-making used the diagonal matrix elements of $\hat{H}'$ as the first order corrections to the energies whether the originally chosen basis is a *good* basis or not (whether $\hat{H}'$ in that basis was a diagonal matrix in the degenerate subspace of $\hat{H}^0$ or not).

Interviews also suggest that students with this type of sense-making were often only focused on the mathematical expressions for the first order perturbative corrections in Eqs. 1 and 2 (e.g., if an expression has a denominator that is zero) and did not reflect upon the fact that these energy corrections are only meaningful for a *good* basis. They also did not realize that a basis that cannot be used to find corrections to the energy eigenstates is not valid for finding corrections to the energies either.

3. *Mathematics instantiated incorrectly in the physics context*

Choosing different bases for different parts of the same problem: Some interviewed students struggled to identify $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$. This was especially true in examples in which the basis states for the unperturbed Hamiltonian and perturbation matrices were such that the degenerate states were not in adjacent rows/columns. In Q7, students needed to exercise caution when identifying the perturbation in a given degenerate subspace of the unperturbed Hamiltonian $\hat{H}^0$. Choosing the basis states in a particular order can make it easier to identify the degeneracy in the unperturbed energy spectrum and also identify the perturbation matrix $\hat{H}'$ in each degenerate subspace of the unperturbed Hamiltonian $\hat{H}^0$. In particular, a convenient choice of basis states is one in which the states that share the same energy in the unperturbed Hamiltonian $\hat{H}^0$ are listed in

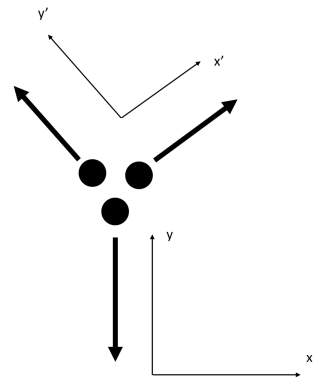

FIG. 3. A common system encountered in introductory physics involving a bomb that explodes into three pieces.

adjacent rows/columns. Regardless of the order in which the basis states are expressed, the first-order corrections to the energies are the same. Choosing basis states in a different order simply changes the order in which the unperturbed energies and the first-order corrections appear as diagonal matrix elements of the $\hat{H}^0$ and $\hat{H}'$ matrices, respectively.

However, interviews suggest that some students struggled to realize that one is free to reorder the basis states without changing the first-order corrections to the energy spectrum but all matrices must be reordered appropriately. For example, one interviewed student claimed that, “We cannot change the order of the basis states since the diagonal (matrix) elements of the perturbation are the first-order corrections to the energy. If we change the order, we change the first-order corrections.” This student did not recognize that changing the order of the basis states for the perturbation matrix would entail that we also rearrange the matrix elements of the unperturbed Hamiltonian $\hat{H}^0$ matrix accordingly. This student and others with this type of reasoning did not consider that changing the order of the basis states simply rearranges the unperturbed energies as the diagonal matrix elements and the corresponding first-order corrections. In other words, reordering of the basis states should be done for both the unperturbed Hamiltonian and the perturbation so it amounts to rearranging the order in which the unperturbed energies appear as the diagonal matrix elements of $\hat{H}^0$ and the first-order corrections to those unperturbed energies will still correspond to the same unperturbed energies.

Interviews suggest that students with this type of struggle in sense-making focused on the mathematics and the matrices separately without reflecting upon the fact that the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation $\hat{H}'$ must be considered together in order to determine the perturbative corrections. While sense-making, they did not realize that matrix elements corresponding to the unperturbed energies and the first order corrections to the energies are in the same position in the two matrices only when the basis states are chosen in the same order for both matrices. During individual discussions, some students who were specifically asked to draw their attention to the fact that both the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation $\hat{H}'$ must be considered together noted that they did not know why the order of the basis states should be changed in both when only one of the matrices did not have the degenerate states in the adjacent rows/columns.

An analogous challenge in introductory physics is students being inconsistent across different parts of a problem [129]. For example, one inconsistency in introductory physics is students mixing up different coordinate systems or using different coordinate systems for different parts of the same problem without reconciling the differences before comparing the different parts of the problem. For example, a common problem from introductory physics involves applying conservation of linear momentum when an object explodes. A diagram for this type of problem is depicted in Fig. 3. One type of inconsistency displayed in this type of problem is that students choose two coordinate systems, such as the $x - y$ and $x' - y'$ coordinate systems in Fig. 3. After considering the momentum of each the pieces in these two different coordinate systems, some students incorrectly equate the momenta in the x and x' direction and the momenta in the y and y' direction, rather than choosing a single coordinate system and expressing each momentum vector in terms of the components in that coordinate system. Even in intermediate mechanics, students may combine or mix up Cartesian and polar coordinate systems, e.g., while solving a simple pendulum problem in a way that they end up with an equation that is dimensionally incorrect using Newton’s second law (dimensions of force on one side of the equation and mass times the second derivative of an angle with respect to time on the other side) [135].

Below, we discuss two types of student responses that demonstrate that these advanced students struggled to choose a consistent representation for the unperturbed Hamiltonian $\hat{H}^0$ and the perturbation $\hat{H}'$ and had difficulty making the connection between these two operators.

Reasoning primitive “everything matters” manifests as one must diagonalize the entire $\hat{H}'$ matrix instead of just a subspace in which $\hat{H}^0$ has degeneracy: Some students did not realize that $\hat{H}'$ can be diagonalized in each degenerate subspace of $\hat{H}^0$ while keeping $\hat{H}^0$ diagonal even when $\hat{H}^0$ and $\hat{H}'$ do not commute.

For example, in Question Q6(a), one student in the interview stated, "We cannot diagonalize a part of $\hat{H}'$, we must diagonalize the whole thing." Interviews suggest that students sometimes thought that the entire perturbation Hamiltonian must be diagonalized. Their sense-making did not account for the fact that the degeneracy in the eigenvalue spectrum of $\hat{H}^0$ provides flexibility in the choice of basis in the degenerate subspace of $\hat{H}^0$ so that $\hat{H}'$ can be diagonalized in that subspace (even if $\hat{H}^0$ and $\hat{H}'$ do not commute) while keeping $\hat{H}^0$ diagonal. For example, if we consider the case in which $\hat{H}^0$ has a two-fold degeneracy, then $\hat{H}^0\psi_a^0 = E^0\psi_a^0,\ \hat{H}^0\psi_b^0 = E^0\psi_b^0,$ and $\langle\psi_a^0|\psi_b^0\rangle = 0$ where ψ_a^0 and ψ_b^0 are normalized degenerate eigenstates of $\hat{H}^0$. Any linear superposition of these two states, e.g. $\psi^0 = \alpha\psi_a^0 + \beta\psi_b^0$ with $|\alpha|^2 + |\beta|^2 = 1$, is an eigenstate of $\hat{H}^0$ with the same energy E^0. Some interviewed students did not realize that since any linear superposition of the original basis states that correspond to the degenerate subspace of $\hat{H}^0$ remains an eigenstate of $\hat{H}^0$, one can choose that special linear superposition that diagonalizes $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$.

Interviews suggest that some students with this type of sense-making thought that it was not possible to only diagonalize part of the $\hat{H}'$ matrix while keeping $\hat{H}^0$ diagonal. Some students relied on their mathematical intuition to incorrectly claim that changing bases to diagonalize $\hat{H}'$ in the degenerate subspace of $\hat{H}^0$ would also affect the $\hat{H}^0$ matrix. These interviewed students sometimes referenced a problem from one of their mathematics courses in which they had two matrices and that after performing a change of basis, the two matrices must be different in the new basis compared to the matrices in the initial basis. While this type of reasoning is correct for the case in which there is no degeneracy in the energy spectrum of either $\hat{H}^0$ or $\hat{H}'$, these students did not realize that when there is degeneracy in the unperturbed energy spectrum, the unperturbed Hamiltonian in the degenerate subspace is identical in any basis consisting of states that make up any linear combinations of states with the same energies.

Reasoning primitive "part represents whole" manifests as a *good* basis for one of the terms in the perturbation must be a *good* basis for the entire perturbation: Interviews suggest that some students with this type of sense-making used reasoning that was locally consistent, but they were not reasoning holistically and did not recognize that their answer was not globally consistent. For example, some students who correctly considered both $\hat{H}^0$ and $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ when determining a *good* basis for the perturbative corrections of the hydrogen atom placed in an external magnetic field for the Zeeman effect still struggled in identifying a *good* basis for perturbative corrections. Since $\hat{H}'_{fs}$ is diagonal in each degenerate subspace of $\hat{H}^0$ if a basis consisting of states in the coupled representation is chosen and $\hat{H}'_Z$ is diagonal if a basis consisting of states in the uncoupled representation is chosen, but not vice versa, neither basis forms a *good* basis for the Zeeman effect. For example, in question Q3, some students correctly identified that the *good* basis for the fine structure term $\hat{H}'_{fs}$ is a basis consisting of states in the coupled representation (option i) and also correctly identified that the *good* basis for the Zeeman term $\hat{H}'_Z$ is a basis consisting of states in the uncoupled representation (option ii in Q3). However, after correctly identifying the *good* basis for each of the two perturbations individually, they did not correctly identify that neither the coupled nor the uncoupled representation (option v in Q3) form a *good* basis for the Zeeman effect in which $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$. One interviewed student reasoned that "the coupled [representation states] are a *good* basis for $\hat{H}'_{fs}$ and uncoupled [representation states] are a *good* basis for $\hat{H}'_Z$, so both coupled and uncoupled form a *good* basis for $\hat{H}'_{fs} + \hat{H}'_Z$."

Interviews suggest that students with this type of sense-making thought that since a basis consisting of states in the coupled representation (option i in Q3) is a *good* basis for the fine structure term $\hat{H}'_{fs}$ and a basis consisting of states in the uncoupled representation (option ii in Q3) is a *good* basis for the Zeeman term $\hat{H}'_Z$, then either basis is a *good* basis for the perturbation consisting of the sum of these two terms. These students did not reflect upon the fact that the uncoupled representation is not a *good* basis for $\hat{H}'_{fs}$ and therefore cannot be a *good* basis for the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$. They also did not realize that the coupled representation is not a *good* basis for $\hat{H}'_Z$ and cannot be a *good* basis for the perturbation $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$.

4. *The term "linear combination" of states activates different novice-like knowledge resources from different students*

Student sense-making in the interviews suggests that some students struggled to realize that it is generally not the case that a linear combination or linear superposition of energy eigenstates is an energy eigenstate. It is only true that a linear combination of energy eigenstates is an energy eigenstate when all of the states share the same energy. However, they were overgeneralizing a familiar example and did not recognize the inconsistency in their reasoning. Different students used different reasoning primitives concerning linear combinations of states. One reasoning primitive some students used is that combining things maintains features so a linear combination of energy eigenstates must be an energy eigenstate (superposition maintains eigenstate). The other reasoning primitive some students used is that combining things destroys feature so a linear combination of energy eigenstates can never be an energy eigenstate (superposition destroys eigenstate). Below, we discuss each of these two types of student sense-making.

Reasoning primitive "combining things maintains features" manifests as a linear combination of energy eigenstates MUST be an energy eigenstate: Some students incorrectly claimed that the linear combination (superposition) of energy eigenstates must be an energy eigenstate. In general, it is not the case that a linear combination of energy eigenstates must be an energy eigenstate (while it is true for problems involving DPT in which the degeneracy in the energy spectrum allows for certain linear combination to be energy eigenstates). Interviews suggest that oftentimes, students with this type of sense-making did not explicitly work through the mathematics of the TISE to check that a state consisting of a linear combination of energy eigenstates satisfies the TISE. If they had, the result of the operator acting on the linear combination of eigenstates with different energies would not have returned a constant multiplied by the same linear combination. A similar difficulty has been found in prior investigations [98] in other contexts when students were asked to consider two stationary states, ψ_1 and ψ_2, for the TISE $\hat{H}\psi = E\psi$, such that $\hat{H}\psi_1 = E_1\psi_1$ and $\hat{H}\psi_2 = E_2\psi_2$. In that study, some students had a tendency to overgeneralize the TISE $\hat{H}\psi = E\psi$ and claimed that if ψ_1 and ψ_2 are stationary states, then their linear combination $\psi_1 + \psi_2$ will also be a stationary state. However, in general, $\hat{H}(\psi_1 + \psi_2) = E_1\psi_1 + E_2\psi_2 \neq E(\psi_1 + \psi_2)$ unless there is a degeneracy in the energy spectrum so that $E = E_1 = E_2$.

For example, in Q2, in the context of the hydrogen atom placed in an external magnetic field, some students correctly stated that a basis consisting of states in the uncoupled representation makes the operator $\hat{H}'_Z$ diagonal in each degenerate subspace of $\hat{H}^0$, but then went on to incorrectly claim that any arbitrary linear combination of states in the uncoupled representation also makes the operator $\hat{H}'_Z$ diagonal in each degenerate subspace of $\hat{H}^0$. Students with this type of reasoning selected both options ii and iv in Q2. During an interview, one student who selected options ii and iv for $\hat{H}'_Z$ incorrectly reasoned: "If the uncoupled [states] are eigenstates [of $\hat{H}'_Z$] then so is their linear combination." In general, it is not true that linear combinations of states in the uncoupled representation are eigenstates of $\hat{H}'_Z$ (although certain special linear combinations of states in the uncoupled representation remain eigenstates of $\hat{H}'_Z$ due to the degeneracy). Similar reasoning was sometimes used by students who selected both options i and iii on Q2 for the operator $\hat{H}'_{SO}$.

Reasoning primitive "combining things destroys features" manifests as a linear combination of energy eigenstates can NEVER be an energy eigenstate: When there is degeneracy in the energy spectrum, it is the case that a linear combination of energy eigenstates that have the same energy is also an energy eigenstate. Some students claimed that a linear combination of degenerate states cannot be an energy eigenstate. Students with this type of sense-making struggled with the fact that the linear combination of eigenstates is an eigenstate if the eigenstates have the same eigenvalue. During the interview, they often incorrectly reasoned that a linear combination of energy eigenstates cannot be an eigenstate without doing an explicit calculation to ensure that the linear combination is an energy eigenstate for degenerate states.

Some interviewed students cited a common example they were familiar with, e.g., of the one-dimensional infinite square well. In that situation, because there is no degeneracy in the energy spectrum of the one-dimensional infinite square well, a linear combination of energy eigenstates is not an energy eigenstate. For example, a linear combination of the ground state and the first-excited state is not an energy eigenstate of the one-dimensional infinite square well. Recalling these types of facts, some interviewed students incorrectly overgeneralized this result to cases in which there is a degeneracy in the energy spectrum. In the context of DPT, if a linear combination of states is constructed from energy eigenstates that all share the same energy, then this particular linear combination is an energy eigenstate. Again, even during interviews, students did not work out the mathematics on their own to show that this is true.

Thus, students with this type of reasoning were overgeneralizing the case in which a linear combination of non-degenerate energy eigenstates is not an energy eigenstate to imply that a linear combination of energy eigenstates is never an energy eigenstate. These students struggled to connect that it is the degeneracy in the unperturbed energy spectrum that allows one to determine a *good* basis in the context of DPT. If the initial basis is not a *good* basis, one must find a linear combination of the unperturbed energy eigenstates that diagonalize the perturbation $\hat{H}'$ in each degenerate subspace of $\hat{H}^0$ while ensuring that the *good* basis is a complete set of eigenstates of $\hat{H}^0$.

C. Challenges in performing self-monitoring and checking to identify inconsistencies in one's reasoning

The following three types of sense-making and reasoning show that these advanced students are still developing expertise and because their knowledge of relevant concepts is fragmented, they either failed to make connections between related problems or did not perform necessary check to identify inconsistencies in their answers. While some examples of not performing consistency checks are discussed in earlier sections, here we focus specifically on these issues in cases where students provided inconsistent answers to questions with similar themes or did not do reasonability check for their answers.

Calculating non-zero off-diagonal matrix elements of a given operator in one problem and proceeding to claim that the operator was diagonal in the same basis in a later problem: Students were asked to determine several diagonal and off-diagonal matrix elements for the operators $\hat{H}'_{SO}$ and $\hat{H}'_Z$ in both the coupled and uncoupled representations. Some students calculated non-zero off-diagonal matrix elements for an operator in a given basis and in a subsequent problem stated that the same operator is diagonal in that basis. For example, students were asked to calculate an off-diagonal matrix element of $\hat{H}'_{SO}$ in which the basis was chosen in the uncoupled representation. Some students correctly calculated this non-zero off-diagonal matrix element, but then in Q2 chose the uncoupled representation as a basis in which the spin orbit term $\hat{H}'_{SO}$ is diagonal. These students either did not self-monitor to identify the inconsistency in their responses or did not realize the connection between the two problems.

Students with these types of responses did not connect the results of their mathematical calculations in one problem to a more conceptual question later in the same assessment. Some of the interviewed students with this type of reasoning did not activate relevant knowledge (even if they had it) to interpret the mathematical expressions, e.g., in Q1 (and other similar expressions) as matrix elements associated with diagonal and off-diagonal matrix elements of the operators $\hat{H}'_Z$ and $\hat{H}'_{SO}$. Interviews suggest that some of them simply calculated the expressions and did not reflect upon why they were asked to perform such calculations and how these expressions were helpful overall in the context of DPT.

Challenges in identifying and monitoring whether the answers are vector or scalar quantities: Calculating suitable matrix elements in different bases is an important step in many DPT problems. In order to be able to determine a *good* basis, one must determine a basis in which the unperturbed Hamiltonian is a diagonal matrix and the perturbation matrix $\hat{H}'$ is diagonal in each degenerate subspace of $\hat{H}^0$. To probe whether students were able to determine matrix elements for operators involved in the hydrogen atom in an external magnetic field, they were asked to determine several diagonal and off-diagonal matrix elements for various operators in different bases. We find that students struggled to correctly determine these matrix elements. Additionally, some interviewed students immediately began by writing down equations that they thought were needed to calculate the matrix elements and launched into a complex calculation to solve them rather than first analyzing the situation to determine whether explicit calculations were even necessary or whether the matrix elements were zero based upon some conceptual consideration that did not require calculations.

When asked to determine the mathematical expression in Q1(a) and Q1(b), some students struggled to realize that these are matrix elements whose values are constants. Some students, instead, incorrectly evaluated the expression in Q1(a) and Q1(b) as a vector quantity. For example, in Q1(b), one student incorrectly wrote the expression $\langle 2,1,\frac{1}{2},1,\frac{1}{2}|(\vec{S}\cdot\vec{L})|2,1,\frac{1}{2},-1,\frac{1}{2}\rangle = \frac{\hbar^2}{2}|2,1,\frac{1}{2},-1,\frac{1}{2}\rangle$. Students with this type of response struggled to connect the matrix elements of the perturbation $\hat{H}'$ to values of the energy correction which is not a vector quantity. These types of challenges are also observed among introductory physics students, e.g., they sometimes struggle to identify whether the solution to a problem is a vector or scalar quantity [136–138]. For example, some introductory students incorrectly identify that the dot product of two vectors results in a vector quantity [136–138].

For Q1(a) and Q1(b), some students only focused on the operator acting on the ket state and appropriate resources related to the inner product of the bra and ket states were not activated even if they knew them as evidenced by their other responses. The basis states in the coupled representation are orthonormal (and similarly in the uncoupled representation). For example, the following is one student's response after traditional lecture-based instruction for Q1(b):

$$\begin{aligned}(\vec{S}\cdot\vec{L})|2,1,\tfrac{1}{2},-1,\tfrac{1}{2}\rangle &= [\tfrac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z]|2,1,\tfrac{1}{2},-1,\tfrac{1}{2}\rangle \\ &= \tfrac{1}{2}[\hbar^2\sqrt{2}\sqrt{1}]|2,1,\tfrac{1}{2},0,-\tfrac{1}{2}\rangle \\ &\quad +(-1)(\tfrac{1}{2})\hbar^2|2,1,\tfrac{1}{2},-1,\tfrac{1}{2}\rangle \\ &= \tfrac{\hbar^2\sqrt{2}}{2}|2,1,\tfrac{1}{2},0,-\tfrac{1}{2}\rangle - \tfrac{\hbar^2}{2}|2,1,\tfrac{1}{2},-1,\tfrac{1}{2}\rangle.\end{aligned}$$

The student's final answer for Q1(b) was $\hbar^2[\frac{\sqrt{2}}{2}-\frac{1}{2}]$. All the steps in the above calculation are correct. However, when taking the inner product with the bra state, both terms in the above expression are zero as the inner product $\langle 2,1,\frac{1}{2},1,\ -\frac{1}{2}|2,1,\frac{1}{2},0,\ -\frac{1}{2}\rangle = 0$ and $\langle 2,1,\frac{1}{2}\ 1,\ -\frac{1}{2}|2,1,\frac{1}{2},\ -1,\ \frac{1}{2}\rangle = 0$. Thus, the correct answer is that the matrix element is zero.

This student and others who made similar mistakes did not consider the inner product between the bra and ket states. Students with this type of response did not activate the resource that the first-order corrections to the energies in DPT are the expectation values of the given perturbation and that the calculation of the expectation value always requires the inner product of the bra and ket state. A similar situation occurs when introductory physics students solve problems and may not recognize that their units are dimensionally inconsistent with the requested quantity or change the units (or sign) to match the physical quantity they were supposed to find without correcting the mistake that gave rise to the dimensional and other inconsistencies [68, 139, 140]. For example, many introductory physics students agree with the statement that "momentum is a force" [139] even though this statement is dimensionally incorrect while other introductory students may change the sign of a physical quantity in an equation to suit their intuition [68, 140] when solving problems (without doing a deeper reflection on why the sign issues arose in the first place, e.g., if the square of the speed turned out to be negative [68]).

Choosing a basis that makes the operators $\hat{H}^0$ and $\hat{H}'$ diagonal but not choosing that same basis as a *good* basis for finding the corrections to the energies: Some students did not realize that a basis that makes both $\hat{H}^0$ and $\hat{H}'$ diagonal is a *good* basis for DPT. These students often answered Q2 correctly by identifying a basis that makes both $\hat{H}^0$ and $\hat{H}'$ diagonal, but then they incorrectly answered Q3 and did not choose a *good* basis as one that makes both $\hat{H}^0$ and $\hat{H}'$ diagonal. For example, one student correctly chose options i, ii, iii, and iv as representations that make $\hat{H}^0$ diagonal and option i as the representation that makes $\hat{H}'_{SO}$ diagonal in each degenerate subspace of $\hat{H}^0$ in Q2. This same student then incorrectly chose options i, ii, iii and iv as the representations that form a *good* basis in Q3 despite not choosing options ii, iii, and iv as representations that make $\hat{H}'_{SO}$ diagonal in each degenerate subspace of $\hat{H}^0$. Interviews suggest that some students were not self-monitoring and when explicitly asked to consider their different responses, they were able to reconcile their differences. However, other interviewed students still did not identify their inconsistent responses in Q2 and Q3. These students used correct reasoning from some of the perturbations listed in Q2 and Q3, but did not apply this correct reasoning to all of the listed perturbations.

This type of inconsistency in solving similar problems has been observed in prior research in introductory physics, e.g., in which students are asked to write a mathematical expression for the electric field and plot the electric field as a function of the distance from the center of a sphere [113]. In that study, students often relied upon a mathematical expression rather than their correct physical intuition. For example, one student correctly stated that the electric field inside a solid conducting spherical shell of inner radius b and outer radius c is zero, but then later when asked for a mathematical expression for the electric field wrote the expression $E = -4\pi c^2 + 4\pi b^2$ which is nonzero since $b \neq c$ (it is also dimensionally incorrect and contains no parameters related to electricity). Students in that study often used quantitative reasoning in writing the mathematical expression for the electric field and used qualitative reasoning when plotting the electric field. As a result, they often provided contradictory solutions to the same problem via the two approaches without realizing that there was inconsistency between different responses.

D. Other epistemological issues

1. Reliance on memorized information

Some interviewed students who did not have a functional understanding of the operators involved in the Hamiltonian of the hydrogen atom placed in an external magnetic field admitted to memorizing which set of basis states would form a *good* basis in the context of the hydrogen atom placed in an external magnetic field. For example, one interviewed student noted: “I was always confused with coupled and uncoupled representation. I just memorized when to use which.” Memorization of which representation to use in different situations often masked the fact that students did not have a functional understanding of the relevant linear algebra concepts in order to apply them in this QM context.

Additionally, some students during the interview reproduced the memorized equation for the first-order corrections to the energies and energy eigenstates (without looking up) but then struggled to apply these equations appropriately in a problem. Their approach was consistent with the view that physics is a collection of disjointed facts and sets of equations [15].

2. Challenges in connecting the mathematical models with the physical phenomenon and invoking authority

Of the students who correctly identified that a *good* basis for the intermediate field Zeeman effect consists of special linear combinations of states in the coupled representation (or, equivalently, special linear combinations of states in the uncoupled representation), some struggled with the fact that the first order corrections to the energy spectrum would be the same regardless of the initial choice of the basis. Since neither a basis consisting of states in the coupled representation nor a basis consisting of states in the uncoupled representation form a *good* basis, a *good* basis cannot easily be identified at the outset. In order to determine a *good* basis, one can choose a basis consisting of states in the coupled representation and then diagonalize $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ in each degenerate subspace of $\hat{H}^0$ to determine a *good* basis and the first order corrections to the energy spectrum due to the Zeeman effect. However, one could also choose a basis consisting of states in the uncoupled representation and then diagonalize $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ in each degenerate subspace of $\hat{H}^0$ to determine a *good* basis and the first order corrections to the energy spectrum due to the Zeeman effect. Regardless of the choice of the original basis, after diagonalizing $\hat{H}' = \hat{H}'_{fs} + \hat{H}'_Z$ in each degenerate subspace of $\hat{H}^0$, the first order corrections to the energy spectrum due to the Zeeman effect will be the same in ANY *good* basis. Some students thought that the first order corrections to the energies depended on the original choice of basis. They claimed that if one chooses a basis consisting of states in the coupled representation then the first order corrections in this case would be different than the first order corrections obtained had a basis consisting of states in the uncoupled representation been chosen as the original basis.

Some students invoked authority (textbook, instructor etc.), e.g., regarding intermediate field Zeeman energy corrections when asked whether writing the perturbation Hamiltonian in two different initial bases (such as the coupled or uncoupled representation in which it is not diagonal) and then diagonalizing it in each case would yield the same or different corrections to the energy. For example, one student thought that only the coupled representation that was chosen as the initial basis in the textbook may be the correct initial basis to write the non-diagonal perturbation Hamiltonian (e.g., in the n=2 degenerate subspace) before diagnonalizing it to obtain the corrections to the energy but they were not able to explain their reasoning coherently.

Interviews also suggest that students with these types of sense-making patterns often focused on the fact that the matrix elements of the perturbation in a given basis, not necessarily a *good* basis, depend on the initial choice of basis and then incorrectly inferred that the first order corrections would also be different. However, it does not make sense experimentally that the observed perturbative corrections would depend upon the initial choice of basis. Once a *good* basis is determined by diagonalizing the perturbation Hamiltonian starting from an initial basis, the first order corrections to the energies must be the same regardless of the initial choice of basis. Advanced students' lack of connecting mathematics with physical situations in the context of DPT for the Zeeman effect sheds light on the challenges in sense-making in QM.

An expert in quantum mechanics is likely to do sense-making to connect the predictions of the quantum mechanical models and what is observed in the experiments to ensure that there are no inconsistencies. Some advanced students' sense-making shows that they struggled with the fact that the initial choice of basis will not affect what one obtains after diagonalizing the perturbation Hamiltonian since those diagonal values correspond to observed energy shifts (which are physical and observed in the experiments). This struggle while solving DPT problems may be a reflection of the challenges in making appropriate math-physics connection and the fact that advanced students are still developing expertise in this novel domain of QM.

3. Challenge in recognizing the utility of a limiting case in the strong and weak field Zeeman effects and making the connection to the intermediate field Zeeman effect in the appropriate limits

Understanding when and how to make limiting case approximations and why they are valid in a particular situation is a hallmark of expertise in physics. Using limiting cases can simplify the problem-solving process significantly and can provide a means to check that the results obtained are reasonable. Some students struggled to connect these limiting cases to the intermediate field Zeeman effect. They did not realize that under the appropriate limits, the first-order corrections to the intermediate field Zeeman effect for the hydrogen atom are consistent with the first order corrections in the strong and weak field Zeeman effects when using the two-step approximation method. In fact, interviews suggest that some students viewed the limiting cases of the strong and weak field Zeeman effects as entirely separate problems and did not think of these limiting cases as related at all to their previous work on the intermediate field Zeeman effect. In the two-step approximation method for the strong field Zeeman effect, states in the uncoupled representation are chosen as a basis since this choice makes $\hat{H}^0$ and $\hat{H}'_Z$ diagonal. While a basis chosen to be states in the uncoupled representation does not diagonalize $\hat{H}'_{fs}$, this basis does diagonalize both $\hat{H}^0$ and $\hat{H}'_Z$ and we can treat $\hat{H}'_{fs}$ in the second step as the smaller contribution to the corrections to the energy spectrum. In this two-step approximation, $\hat{H}'_{fs}$ only needs to be diagonal in each degenerate subspace after the first step. Some students struggled to identify when it was valid to use the two-step approximation and connect these limiting cases with the intermediate field Zeeman effect in the appropriate limits. When answering Q4, one interviewed student stated, "I like the strong and weak field problems because the uncoupled and coupled representation magically work." Probing shows that some of the students with these challenges did not think that the intermediate field Zeeman effect would give the same corrections to the energy as the strong and weak field Zeeman effect expressions in the appropriate limits. Their sense-making and reasoning shows evidence of fragmented knowledge resources in that some of their assertions were correct but they could not be used to make other related inferences.

V. SUMMARY

Our findings show that some advanced students who had learned relevant concepts in their traditionally taught quantum mechanics courses struggled with sense-making and integrating physics and mathematics concepts in order to solve the DPT problems. In different problem-solving tasks, different knowledge resources got activated even if the same concepts were applicable. Student sense-making and reasoning showed use of different reasoning primitives.

We also find that students in the "physics mode" displayed some behavior somewhat similar to the students playing the mapping meaning to mathematics epistemic game [15], in which they began by creating a story describing the physical situation, but then a disconnect occurred when transitioning to the underlying mathematical concepts [18]. Oftentimes, based upon their physical intuition, this disconnect involved using a reasoning primitive that was only locally consistent. This type of problem solving behavior can be attributed to advanced students' developing expertise in that their knowledge structure in QM is only locally coherent, and their sense-making is not expert-like to the point of recognizing these inconsistencies while solving problems. In some cases discussed, the students only used their physical intuition (or "gut-feeling") while sense-making and did not integrate the physical and mathematical concepts appropriately. Students in the "math mode" used a problem-solving approach that began with an equation and then at the end of the problem solving process they tried to make physical sense of their answer [18]. Oftentimes, students relied on the results of their calculations to make inferences and did not, e.g., reflect upon the fact that their answers were inconsistent with the physical laws because the mathematical process was not correct. In these situations, student sense-making and reasoning often suggested, e.g., that they tended to focus their attention on a single entity or on individual parts of the calculations and did not think more globally about the overall goal of the problem and how the problem can be solved by following a systematic process that starts with conceptual analysis and planning of the solution. In other cases, students appeared not to have a strong background in linear algebra while solving QM problems related to DPT and as a result applied linear algebra concepts incorrectly or used their mathematical intuition when this intuition was not correct for the problem situation. Thus, similar to the case when students are in the physics or math mode in introductory physics context [15], because advanced students are not experts in QM and/or linear algebra, they often did not display expert-like sense-making and recognize the inconsistencies in their sense-making.

Students who did not engage in self-monitoring, regulating, and checking their answers while sense-making often did not identify inconsistencies in their answers and reasoning across contexts. Furthermore, students with other epistemological issues in solving DPT problems often resorted to memorized information, relied on authority, struggled to recognize inconsistencies or make meaningful inferences or struggled to discern the validity and scope of issues related to DPT in different situations. For example, some thought that the initial choice of basis for a matrix representing a perturbation Hamiltonian would determine what the first order corrections to the energies would be after diagonalizing the Hamiltonian. However, if we make connection between the first order corrections to the energies obtained using DPT and experiments, it does not make sense experimentally that the observed perturbative corrections would depend upon the initial choice of basis. In particular, once a good basis is determined by diagonalizing the perturbation Hamiltonian starting from an initial basis, the first order corrections to the energies must be the same regardless of the initial choice of basis. However, deep reflections about these issues regarding connection between corrections to the energies and outcomes of experiments are necessary. Similarly, some students thought that the results for the strong and weak field Zeeman effect cannot match those of the intermediate field Zeeman effect in the appropriate limits because the basis chosen for strong field or weak field Zeeman effect are uncoupled or coupled representations, respectively, whereas it is neither uncoupled nor coupled for the intermediate field Zeeman effect.

Student sense-making and reasoning challenges while solving DPT problems are evidence of advanced students' evolving expertise in the context of the novel paradigm of quantum mechanics and challenges in integrating mathematical and physical concepts appropriately. The advanced students often had analogous patterns of challenges in sense-making and reasoning as those that have been found in introductory physics. While some learning tools on DPT involving Zeeman effect have been developed [106, 107], other future learning tools that take advantage of this research for helping students with expert-like sense-making in the context of DPT will be useful.

ACKNOWLEDGMENTS

We thank the NSF for award PHY-2309260. We are also thankful to David Meltzer and members of the Department of Physics and Astronomy at the University of Pittsburgh (especially R. P. Devaty). Additionally, we thank the students who participated in this research. We have not cited conference proceedings paper if corresponding journal papers are available.

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