Toward a Concept Inventory for Energy Band Theory: Insights from Textbooks and Graduate Exam Syllabi

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Energy band theory is a central topic in upper-division solid state physics and plays a foundational role in semiconductors and material science research. However, no validated concept inventory is currently available to measure students' conceptual understandings of this topic. As an initial step toward assessment development, this study reports a content analysis of four widely used textbooks—two in English and two in Chinese—aimed at identifying core concepts in energy band theory across different sources. Results revealed five key concept categories, common across all texts, including foundational approximations, Bloch's theorem, the nearly free electron model, the tight-binding model, and symmetry operators. We validated these concept categories by comparing them against graduate entrance exam syllabi from three major Chinese universities. The convergence between textbook content and national curricular expectations supports these five concept categories as the focus for assessment. This work lays the foundation for future development of a research-based concept inventory, capable of supporting instruction and learning in upper-level solid state physics.

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I. INTRODUCTION AND BACKGROUND

The quantum industry increasingly values graduates with practical knowledge of quantum systems and solid-state physics, underscoring the need for robust undergraduate preparation in these areas [1]. Energy band theory—a cornerstone of upper division solid-state physics—is essential for understanding the electronic properties of materials. Foundational concepts concerning Bloch's theorem, the nearly free electron model, and the tight-binding model underpin modern condensed matter physics and enable technologies, including semiconductors and quantum devices. The topic is currently being taught to a large student population. For example, in China alone, over 8,900 students registered for the Material Science Subject Tests of the 2024 Graduate School Entrance Exams, administered independently by 17 Chinese universities [2–18]. These tests explicitly cover topics of energy band theory.

The popularity of upper-level undergraduate solid state physics courses is also evident from the high viewership of publicly available online lecture series delivered by world-leading instructors. Several course series—both in English and Chinese—have garnered over 100,000 views [19–21]. Notably, a recent series by Xiaolong Fan (Lanzhou University, December 2023) [19] has already surpassed 220,000 views, highlighting the continued and growing instructional interest in the topic. Among these instructors, Steve Simon (Oxford, 2014) [20] describes Bloch's theorem as "*the underpinning of all of material science,*" and Jingguang Che (Fudan University, 2012) [21] refers to energy band theory as "*the foundation of solid-state electronic theories.*" These statements underscore the central role of energy band theory in solid state physics.

To date, however, no validated concept inventory exists to assess students' understanding of energy band theory. While physics education research has produced several research-based assessments in quantum mechanics, including the Quantum Mechanics Conceptual Survey (QMCS) [23], the Quantum Mechanics Concept Assessment (QMCA) [24], and the Microscopic models of Electric and Thermal Conductivity of Solids METCS inventory [25], these tools either target introductory content or omit key energy band theory concepts altogether.

Faculty have explicitly called for assessments aligned with upper-division learning goals [26], and exploratory studies have identified student difficulties with solid state and condensed matter concepts [27]. However, no instrument specifically addresses energy band theory at the upper-division level.

To bridge this gap, we have started developing a research-validated concept inventory. As demonstrated by previous work [23–25], the development of a validated concept inventory typically involves several stages, including content identification, expert review, item development, cognitive interviews, pilot testing, and statistical validation. *This manuscript represents the first phase of the study, a content analysis of four widely used textbooks in solid state physics to identify core concepts and organize them into concept categories.* We compared the content analysis findings against graduate entrance exam syllabi from three leading Chinese universities, recognized as national benchmarks for undergraduate preparation in China, to ensure curricular relevance.

II. METHODS

We conducted a content analysis of two internationally popular textbooks written in English and two Chinese textbooks widely adopted by leading universities in China. The English texts were *Introduction to Solid State Physics* by Kittel [28] and *Solid State Physics* by Ashcroft & Mermin [29]. The Chinese-language sources were *Solid State Physics* by Huang [30] and *Fundamentals of Solid State Physics* by Yan [31].

Specifically, we focused on chapters covering energy band theory, including discussions of Bloch's theorem, periodic potentials, Brillouin zones, and key models such as the nearly free electron model and the tight-binding model. We analyzed how key concepts were introduced, applied, and sequenced in these texts.

Concepts were initially identified through open reading of each textbook without pre-defined coding categories. Two researchers independently read and annotated the texts, highlighting concepts as they emerged. Through iterative discussions, these emergent ideas were thematically grouped into broader concept categories based on recurring patterns and pedagogical emphasis. Discrepancies or ambiguities in coding were resolved through consensus. While we did not aim to reach a specific threshold of interrater agreement at this stage, future work will incorporate formal measures to assess coding reliability. Concepts appearing in all four sources were prioritized, however those emphasized in at least three textbooks were also retained due to their instructional relevance.

Our selection of textbooks aimed to capture a range of widely adopted texts used in upper-division solid state physics instruction across different regions and time periods. Two of the texts (Ashcroft & Mermin, and Huang) were published in the late 1970s, while the other two (Kittel [latest edition], and Yan) reflect more recent editions or revisions. This selection allows us to observe both enduring themes and evolving pedagogical trends. Nevertheless, we acknowledge that limiting the sample to four textbooks—drawn only from English- and Chinese-language instruction—may limit the generalizability of our findings. Future work will incorporate additional sources from other regions and modalities (e.g., online course materials) to capture a broader instructional landscape.

To further validate our concept set, we cross-referenced our coded categories with publicly available graduate entrance exam syllabi on solid state physics from three leading Chinese universities: the University of Chinese Academy of Sciences (UCAS) [32], the University of Science and Technology of China (USTC) [33], and the University of Electronic Science and Technology of China (UESTC) [34]. These syllabi outline the expected conceptual preparation for graduate study and shape undergraduate instruction in China. Their alignment with our identified concept categories validates the development framework for the concept inventory.

In this study, we distinguish between concepts and concept categories. A concept refers to a specific principle, approximation, property of a model that represents a distinct unit of disciplinary knowledge. For example, the translational property of wavefunctions under Bloch's theorem is treated as a concept. In contrast, a concept category is a broader thematic grouping that organizes related concepts in textbooks and curricular. For instance, the concept category tight-binding model includes concepts such as its treatment of electrons as localized at lattice sites and its representation of wavefunctions as linear combinations of atomic orbitals.

The resulting set of concepts and concept categories forms the foundation for the next phase of our project, which focuses on developing and validating assessment items through collaboration with both instructors and students.

III. FINDINGS

A. Content analysis of textbooks

The content analysis identified core concepts that were consistently emphasized across all four textbooks and organized them into five concept categories: **foundational approximations**, **Bloch's theorem**, the **nearly free electron model**, the **tight-binding model**, and **symmetry operators**. These concept categories reflect both theoretical foundations and practical models central to energy band theory instruction. Table I summarizes the specific concepts grouped under each category.

TABLE I. Core concepts in energy band theory identified across four textbooks.

Concept Category	Core Concepts Extracted
Foundational Approximations	1. Born–Oppenheimer approximation 2. Single-electron approximation 3. Periodic potential approximation
Bloch's Theorem	1. Wavefunction: $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$ 2. Translation property of the wavefunction: $\psi(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi(\mathbf{r})$; and the lattice translational symmetry of $u_{\mathbf{k}}$: $u_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{\mathbf{k}}(\mathbf{r})$
Nearly Free Electron Model	1. Weak periodic potential treated as a perturbation to the Hamiltonian 2. Band gap formation at Brillouin zone boundaries (1D model)
Tight-Binding Model	1. Electron approximated to be localized at lattice sites 2. Wavefunction approximated as linear combination of atomic orbitals: $\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}\,\phi(\mathbf{r}-\mathbf{R})$
Symmetry Operators	1. Symmetry operator acts on wave functions: $\hat{S}\psi(\mathbf{r}) = \psi'(\mathbf{r})$ 2. The Hamiltonian of a symmetric system commutes with the symmetry operator: $[\hat{H}, \hat{S}] = 0$

1. *Foundational approximations*

We identified the following common set of approximations that serve as the foundation for the development of energy band theory.

- Born–Oppenheimer approximation assumes that electrons move much faster than nuclei, allowing the lattice to be treated as static during electronic motion.
- Single-electron approximation replaces the many-body-electron problem by a mean-field potential, allowing electrons to be treated independently.
- Periodic potential approximation asserts that the effective potential experienced by electrons has the periodicity of the underlying crystal lattice.

All four textbooks explicitly introduce the single-electron and periodic potential approximations within their primary chapters on energy band theory. These concepts are presented as standard modeling assumptions and are deeply integrated into the derivation of electronic wavefunctions and the formulation of energy bands.

The Born–Oppenheimer approximation, however, receives more varied treatment. Yan introduces it explicitly at the beginning of the energy band theory chapter, framing it as a physical prerequisite for separating electronic and lattice problems. Huang, on the other hand, does not include it in the main text of the energy band theory but only provides a summary of all three approximations in the supplementary recitation booklet. Differing from both Yan and Huang, Ashcroft & Mermin discuss the Born–Oppenheimer approximation in a much later chapter (Chapter 22) under the context of classical lattice dynamics, without any explicit connections to the band theory in the earlier chapter (Chapter 8). Yet, Kittel only implicitly embeds the Born-Oppenheimer approximation in the discussion on treatment of electrons moving in a fixed periodic potential.

Despite the variation, a shared emphasis is clearly placed on the single-electron and periodic potential approximations. Although the Born–Oppenheimer approximation is not discussed in the energy band theory chapters by three of the texts, its inclusion in later chapters and supplementary materials suggests that we should recognize its foundational role in energy band theory.

2. *Bloch's theorem*

All four textbooks present Bloch's theorem as the mathematical foundation for describing electron wavefunctions in a periodic potential. The theorem states that the eigenfunctions of the Hamiltonian take the following form:

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\, u_{\mathbf{k}}(\mathbf{r}) \tag{1}$$

where $\mathbf{r}$ is the position vector of an electron, and $\mathbf{k}$ is the crystal wavevector that labels the electron's quantum state, and $u_{\mathbf{k}}(\mathbf{r})$ is a function that shares the periodicity of the lattice:

$$u_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{\mathbf{k}}(\mathbf{r}), \text{for any lattice vector } \mathbf{R}. \tag{2}$$

This structure leads to a key property of the wavefunction, such that under a lattice translation, the wavefunction acquires only a phase factor:

$$\psi_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\, \psi_{\mathbf{k}}(\mathbf{r}), \tag{3}$$

Ashcroft & Mermin, Huang, and Yan each provide a full derivation of this mathematical form by showing that the Hamiltonian commutes with the lattice translation operator. By contrast, Kittel presents the result without any derivation; instead, he only states the wavefunction form and discusses its transformation properties under translation.

In terms of sequencing the topics, Ashcroft & Mermin and Yan introduce Bloch's theorem early, before presenting specific models, such as the nearly free electron model. In contrast, Huang and Kittel introduce Bloch's theorem only after developing the nearly free electron model.

Despite the differences in mathematical treatment and topic sequencing, all four textbooks underscore the essential role of Bloch's theorem in understanding the structure of electronic states in solids.

3. *Nearly free electron (NFE) model*

The nearly free electron (NFE) model is introduced in all four textbooks as a conceptual bridge linking the free electron model and the formation of energy bands in solids. It idealizes electrons as nearly free particles perturbed by a weak periodic potential from the crystal lattice. This model explains the opening of energy gaps at Brillouin zone boundaries due to Bragg reflection, a mechanism that transforms a continuous free-electron energy spectrum into discrete bands.

Kittel and Huang introduce the NFE model before Bloch's theorem, consistent with the idea that the perturbative approach does not require prior knowledge of Bloch's theorem. They begin with the free electron model by introducing the periodic potential as a weak correction, which leads directly to energy gap formation at zone boundaries.

Conversely, Yan and Ashcroft & Mermin present the nearly free electron (NFE) model after introducing Bloch's theorem by focusing on different aspects of the theory. Yan emphasizes the conceptual role of symmetry, explaining how breaking lattice translation symmetry leads to the formation of energy bands and the lifting of degeneracy. In contrast, Ashcroft & Mermin focus on a mathematical treatment, applying the perturbation theory to a weak periodic potential to calculate band splitting near Brillouin zone boundaries, without explicitly addressing symmetry in their discussion.

Across all four textbooks, the NFE model is consistently used to explain the band formation as a result of periodicity and illustrate the origin of energy gaps. Clearly, the pedagogical role of NFE in linking simple electron models to realistic band structures supports its inclusion as a core concept category for assessment.

It is worth noting that the sequencing of the NFE model and Bloch's theorem does not appear to correlate with a textbook's publication date. For example, Kittel (2018 edition) and Huang (1979) both present the NFE model prior to Bloch's theorem, whereas Ashcroft & Mermin (1976) and Yan (2000) introduce Bloch's theorem first. This pattern suggests that the ordering of topics reflects differing instructional priorities rather than the era in which the textbooks were written.

4. *Tight-binding (TB) model*

The tight-binding (TB) model emerged as a key concept category, comprising related concepts that are consistently presented across all four textbooks. This model depicts electrons as being localized at lattice sites. In contrast to the nearly free electron (NFE) model, which treats the periodic potential as a weak perturbation to the Hamiltonian, the TB model begins by assuming the electron wavefunction as a linear combination of atomic orbitals (LCAO).

In this model, the electron is tightly bound to atoms, and energy bands arise from weak overlaps between adjacent orbitals. The wavefunction is expressed as the following:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}\, \phi(\mathbf{r}-\mathbf{R}), \tag{4}$$

where $\phi(\mathbf{r}-\mathbf{R})$ is wavefunction of an atomic orbital localized at lattice site $\mathbf{R}$.

All four textbooks—Ashcroft & Mermin, Kittel, Yan, and Huang—introduce the tight-binding model by presenting a picture in which the electron is localized at lattice sites. Ashcroft & Mermin describe the tight-binding model as one that assumes the bound atomic levels are well localized. From a different perspective, Kittel refers to the TB model as an approximate approach that starts from a linear combination of the wavefunctions of free atoms. With a more refined explanation, Yan proposes that when orbital overlaps are small, the wavefunction can be viewed as a linear combination of degenerate atomic orbitals. Similarly, Huang notes that near each lattice site, the electron behaves like being in a state bound to the atom.

In summary, all four textbooks use the tight-binding model to describe how energy bands can emerge from localized states in a periodic structure. The consistency in the presentation of concepts within this category justifies its inclusion as a core concept category for our assessment instrument.

5. *Symmetry Operators*

Three of the four textbooks—Ashcroft & Mermin, Huang, and Yan—explicitly introduce symmetry operators in the context of Bloch's theorem and wavefunction behavior in periodic systems. These treatments emphasize two key principles:

- Symmetry operations are defined by how wavefunctions transform, typically expressed as $\hat{S}\psi(\mathbf{r}) = \psi'(\mathbf{r})$, where $\hat{S}$ indicates a symmetry operation such as lattice translation or rotation.
- If a system exhibits a physical symmetry, its Hamiltonian commutes with the corresponding symmetry operator, $[\hat{H}, \hat{S}] = 0$, which is equivalent to $\hat{S}^\dagger \hat{H} \hat{S} = \hat{H}$.

These principles are used to justify the form of Bloch wavefunctions as eigenstates of both the Hamiltonian and lattice translation operators. Ashcroft & Mermin, Huang, and Yan all use this formalism in their derivation and justification of Bloch's theorem.

The consistent use of symmetry-based discussion in the three major texts supports the inclusion of symmetry operations as a core concept category for the assessment instrument.

B. Alignment with graduate entrance exam syllabi

To further validate the relevance of these concept categories identified from the above textbook analysis, we reviewed publicly available graduate entrance exam syllabi on solid state physics from three leading Chinese universities: the University of Chinese Academy of Sciences (UCAS) [32], the University of Science and Technology of China (USTC) [33], and the University of Electronic Science and Technology of China (UESTC) [34]. These syllabi represent national curricular benchmarks and outline the expected conceptual preparation for graduate-level study in physics.

All three syllabi explicitly require the knowledge of three core categories identified in our previous analysis:

- Bloch's theorem
- Nearly free electron model
- Tight-binding model

Each syllabus requires not only students' familiarity with concepts within these categories but also the ability to apply them in problem-solving. The UCAS and UESTC further require student understanding of the physical processes underlying the theorem and the models.

While foundational approximations and symmetry operators are not listed as standalone categories in these syllabi, they play a foundational role in supporting the three concept categories that are explicitly named. The periodic potential assumption, single-electron approximation, and symmetry-based derivation of Bloch's theorem are essential to the formulation and application of both the NFE and TB models. Their presence across the textbooks, along with their foundational role in supporting the explicitly listed concept categories, justifies their inclusion as core concept categories.

These results confirm that the five concept categories—foundational approximations, Bloch's theorem, the NFE model, the TB model, and symmetry operators—are not only consistently presented across our surveyed textbooks but also align with the national curricular expectations. This convergence clearly indicates that concepts from these categories are centerpieces for teaching energy band theory and ought to be included for assessment development.

IV. CONCLUSION AND FUTURE WORK

This study identified a set of core concepts and concept categories in energy band theory by analyzing four widely used solid state physics textbooks—two in English and two in Chinese. Despite some differences in the sequencing and presentation of these concepts, the textbooks consistently emphasized five key concept categories: (1) foundational approximations, (2) Bloch's theorem, (3) the nearly free electron model, (4) the tight-binding model, and (5) symmetry operators.

To further validate the relevance of these concept categories, we compared our textbook analysis findings against graduate entrance exam syllabi from three leading Chinese universities. These syllabi consistently include Bloch's theorem, the nearly free electron model, and the tight-binding model as required categories. While foundational approximations and symmetry operators are not explicitly named in the syllabi, they play a foundational role in supporting the theorem and models that are explicitly listed. This alignment confirms that the identified concept categories reflect both instructional priorities and formal curricular expectations.

These findings provide a well-supported content foundation for developing a research-based concept inventory of energy band theory at the upper-division undergraduate level. Building on the strong alignment between textbook content and curricular expectations, this set of concepts and concept categories offers a clear and credible basis for assessment development.

In the next phase of this work, we will develop multiple-choice and open-ended items targeting these concepts and concept categories. These items should focus on conceptual understanding of foundational topics—such as the periodic nature of Bloch's theorem, the meaning of key approximations, and the conceptual differences between the nearly free electron and tight-binding models—rather than problem-solving. Items will be refined through physics faculty input and cognitive interviews with students to evaluate their clarity, alignment with the identified core concepts, and diagnostic value. Ultimately, we aim to produce a validated instrument that supports instructors in diagnosing student understanding, comparing curricular approaches, and improving instruction in upper-level solid state physics courses.

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