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Effective interaction in unified perturbation theory

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ABSTRACT

We present a unified description of the Bloch and Rayleigh–Schrödinger perturbation theories of the effective interaction in both algebraic and graphic representations.

1. Introduction

The effective interaction has been an important concept in various quantum many-body problems [1–17]. We first divide a large Hilbert space into a model space (P-space) of a tractable size and its complement (Q-space). Then we define the effective interaction v in the P-space to describe a set of selected eigenstates of the full Hamiltonian H.

There are two different theories to derive the perturbation expansion of v, i.e., the Bloch [7–9] and the Rayleigh–Schrödinger (RS) [17] theories. Though both theories have their own algebraic (bracketing) and graphic (folded diagram) representations for v, their interrelation has not been clarified to date in either representation.

In this uncomfortable situation, we present a unified description of the Bloch and RS perturbation theories in both algebraic and graphic representations generally in nondegenerate P-space. We present the above scenario in the following three steps. The first step describes the Bloch perturbation theory strictly in terms of the "effective transition potential" u between the P- and Q-spaces. At this step, the Bloch perturbation theory acquires its precise description which compares well with the RS counterpart. The second step introduces the "sequence representation" which is a translator between

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the Bloch and RS theories. Here, we also derive the "main frame expansion" which presents v in a simple form that leads directly to both Bloch and RS expansions. The last step derives the Bloch and RS perturbation theories in parallel using the main frame expansion in the sequence representation. The above derivation proves the "unified representation" which exhibits both perturbation theories simultaneously, clarifying their interrelation.

The present work is organized as follows. In Section 2, we describe the effective interaction v fixing the notation. In Section 3, we reconstruct the Bloch theory in terms of the effective transition potential u. In Sections 4 and 5, respectively, we explain the algebraic (bracketing) and graphic (folded diagram) representations for u, which are then summarized in Section 6. Then, by translating the above results for u into those for v, we establish the precise description of the Bloch perturbation theory of v in Section 7. Next, we set out to unify the perturbation theories. In Sections 8 and 9, we introduce the sequence representation and the main frame expansion, respectively. In Sections 10 and 11, respectively, we derive the Bloch and RS perturbation theories of v via the main frame expansion in the sequence representation. In Section 12, we introduce the unified representation which presents these two perturbation theories in a unified fashion in both algebraic and graphic ways, as summarized in Fig. 43. In Section 13, we compare the present approach based on the Bloch theory with the standard RS approach based on the expansion of propagators, to confirm great advantages of the present approach. Finally in Section 14, we summarize the present work.

2. Effective interaction

In this section, we briefly review the effective interaction v using the notation of Refs. [10–12,17].

2.1. Model space

We describe a quantum system in a Hilbert space of dimension D with the following Hamiltonian:

$$H = H_0 + V, \tag{1}$$

where H_0 is the unperturbed Hamiltonian and V is the perturbation. By diagonalizing the full Hamiltonian H in the whole Hilbert space, we obtain D eigenstates of H. In many cases, however, the above diagonalization is beyond the current computer capacity, and we are not usually interested in all of the D eigenstates. Therefore, we divide the Hilbert space of dimension D into a model space (P-space) of tractable dimension d and its complement (Q-space); we are to describe the physics in the d-dimensional P-space. The projection operators onto these spaces are denoted as P and Q, respectively, which satisfy $P^2 = P$, $Q^2 = Q$, and $PQ = QP = 0$. Here we require that the P-space be spanned by a set of d eigenstates $\{|i\rangle,\ i = 1, \dots, d\}$ of H_0 that satisfy

$$H_0|i\rangle = \epsilon_i|i\rangle, \quad i = 1, \dots, d. \tag{2}$$

Then, the Q-space is spanned by the other eigenstates $\{|I\rangle,\ I = d + 1, \dots, D\}$ satisfying

$$H_0|I\rangle = \epsilon_I|I\rangle, \quad I = d + 1, \dots, D. \tag{3}$$

Throughout this work, the P- and Q-space basis states are denoted by lowercase and uppercase letters, respectively. Then the projection operators P and Q are given by

$$P = \sum_{i=1}^{d} |i\rangle\langle i|, \qquad Q = \sum_{I=d+1}^{D} |I\rangle\langle I|, \tag{4}$$

and satisfy the following relations.

$$[H_0, P] = [H_0, Q] = 0, \qquad PHQ = PVQ, \qquad QHP = QVP. \tag{5}$$