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ORIGINAL PAPER

# Effective interactions and block diagonalization in quantum-mechanical problems

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**Abstract** Many models of condensed-matter systems have interactions with unexpected features: for example, exclusively distant-neighbor spin–orbit interactions. On first inspection these interactions seem physically questionable in view of the basis states used. However, such interactions can be physically reasonable if the model is an effective one, in which the basis states are not exactly as described, but instead include components of states removed from the problem. Mathematically, an effective model results from partitioning the Hamiltonian matrix, which can be accomplished by energy-dependent or energy-independent methods. We examine effective models of both types, with a special emphasis on energy-independent approaches. We show that an appropriate choice of basis makes the partitioning simpler and more accurate. We illustrate the method by calculating the spin–orbit splitting in graphene.

**Keywords** Perturbation theory · Partitioned matrix · Hamiltonian matrix · Effective hamiltonian

**Mathematics Subject Classification** 81Q05 · 81Q15

## 1 Introduction

Effective interactions in quantum mechanical problems can lead to models with unusual and counterintuitive features. As an example of current research interest, consider the Kane–Mele model [1] for topological insulators on the hexagonal lattice. This model has two orbitals per atom, one of each spin but both of the same spatial type

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($p_z$). Except for the treatment of the spin–orbit interaction, the Hamiltonian is conventional. The no-spin–orbit part, $\hat{H}_0$, has the usual same-atom and nearest-neighbor interactions. On the other hand, the spin–orbit part, $\hat{H}_{so}$, has only second-near neighbor interactions, with no nearest-neighbor or same-atom terms. The presence of a spin–orbit term in any event is unusual, given that the relevant operator $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}$ has no matrix elements between $p_z$-orbitals of any spins centered on the same atom. Because spin–orbit interactions are nearly always far weaker than those of the main Hamiltonian, $\hat{H}_0$, the exclusively second-near neighbor interactions in $\hat{H}_{so}$ seem on first inspection physically dubious: There are no same-atom or nearest-neighbor spin–orbit interactions, and the most distant couplings in $\hat{H}_0$ are nearest-neighbor.

This apparent dilemma is resolved if one allows the model to be an *implicit effective* one. That is, the $p_z$-orbitals are not simple orbitals; instead, they include the effects of orbitals omitted from the model. The spin–orbit interactions involving the omitted orbitals are thus reflected back into the $p_z$-only model. The model is implicit because it is postulated a priori as opposed to being reduced explicitly from a fully specified Hamiltonian.

Effective models are generally constructed by partitioning the Hamiltonian matrix. Some of the earliest and most familiar methods are based on the work of Löwdin [2–4]. These techniques are often referred to as energy-dependent partitioning because the effective Hamiltonian matrix is energy dependent. Other partitioning methods are energy-independent, often concerned with the perturbation of a degenerate level [5,6]. Yet other energy-independent methods approach the partitioning problem as one of block diagonalizing the Hamiltonian matrix [7–9]. This class of methods is especially useful since the focus is not on a single level, but rather, a smaller Hamiltonian matrix to be subsequently diagonalized. Another method closely related to partitioning is the renormalization method [10].

Here we study block-diagonalization methods for obtaining a smaller effective Hamiltonian matrix. Following a brief review of partitioning methods, we focus on energy-independent block-diagonalization. We show how the conventional energy-independent method can be improved with an appropriate choice of basis, so that the block diagonalization results in a perturbation series of only odd order in the coupling (perturbing) matrix. Thus, in this improved method, solving for each additional term yields an approximation valid to two extra orders of accuracy. We illustrate the method by calculating the effective spin–orbit coupling in graphene and hexagonal (two-dimensional) topological insulators.

## 2 Partitioning methods

### 2.1 General

Suppose that the basis states of the full Hamiltonian can be divided into two classes: class $A$, in which we are interested, and class $B$, which are of lesser interest. The two classes are presumed to be weakly coupled together, and it is usually the case that there are fewer class $A$ states than class $B$ states. The objective is to block diagonalize the Hamiltonian into an effective class-$A$ only Hamiltonian—the effective class-B

Hamiltonian is usually not of interest—up to a desired order in the $A-B$ coupling block. In matrix notation, the full problem reads:

$$\begin{bmatrix} \underline{\mathbf{H}}_{AA} - \underline{\mathbf{1}}_{AA}E & \underline{\mathbf{H}}_{AB} \\ \underline{\mathbf{H}}_{AB}^{\dagger} & \underline{\mathbf{H}}_{BB} - \underline{\mathbf{1}}_{BB}E \end{bmatrix} \begin{bmatrix} \mathbf{v}_A \\ \mathbf{v}_B \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \tag{1}$$

where $\underline{\mathbf{H}}_{cd}$ is size $N_c \times N_d$, $c, d \in \{A, B\}$. Mathematically, the objective is to replace the eigensystem (1) by one in which the diagonal block $\underline{\mathbf{H}}_{AB}$ is zero, or approximately zero.

This may be accomplished in either an energy-dependent or energy-independent manner. When an effective model is constructed explicitly from a fully specified Hamiltonian, either energy-dependent or energy-independent methods may be used. On the other hand, when an effective model is postulated, its Hamiltonian is most often energy-independent (e.g. the Kane–Mele model [1]), meaning that energy-independent partitioning was implicitly assumed.

## 2.2 Energy-dependent partitioning

A brief review of energy-dependent partitioning shows why it can be very useful in constructing explicit effective models but not implicit ones. The energy-dependent partitioning of Eq. (1) can be considered the simplest application of either the Löwdin [2–4] or renormalization [10] methods. Here the method is presented in matrix form; it can also be formulated in terms of operators, as in Löwdin's work [2,4]. Usually the matrix $(\underline{\mathbf{H}}_{BB} - \underline{\mathbf{1}}_{BB}E)$ is nonsingular in the energy range of interest so that the Eq. (1) can be rewritten with the aid of the Schur complement:

$$\begin{bmatrix} \underline{\mathbf{1}}_{AA} & \underline{\mathbf{H}}_{AB}\left(\underline{\mathbf{H}}_{BB} - \underline{\mathbf{1}}_{BB}E\right)^{-1} \\ \underline{\mathbf{0}}_{BA} & \underline{\mathbf{1}}_{BB} \end{bmatrix} \begin{bmatrix} \underline{\mathbf{H}}_{AA} - \underline{\mathbf{1}}_{AA}E - \underline{\mathbf{H}}_{AB}\left(\underline{\mathbf{H}}_{BB} - \underline{\mathbf{1}}_{BB}E\right)^{-1}\underline{\mathbf{H}}_{AB}^{\dagger} & \underline{\mathbf{0}}_{AB} \\ \underline{\mathbf{0}}_{BA} & \underline{\mathbf{H}}_{BB} - \underline{\mathbf{1}}_{BB}E \end{bmatrix} \times \begin{bmatrix} \underline{\mathbf{1}}_{AA} & \underline{\mathbf{0}}_{AB} \\ \left(\underline{\mathbf{H}}_{BB} - \underline{\mathbf{1}}_{BB}E\right)^{-1}\underline{\mathbf{H}}_{AB}^{\dagger} & \underline{\mathbf{1}}_{BB} \end{bmatrix} \begin{bmatrix} \mathbf{v}_A \\ \mathbf{v}_B \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \tag{2}$$

Because the inverse of the left-hand matrix in Eq. (2) exists,

$$\begin{bmatrix} \underline{\mathbf{1}}_{AA} & \underline{\mathbf{H}}_{AB}\left(\underline{\mathbf{H}}_{BB} - \underline{\mathbf{1}}_{BB}E\right)^{-1} \\ \underline{\mathbf{0}}_{BA} & \underline{\mathbf{1}}_{BB} \end{bmatrix}^{-1} = \begin{bmatrix} \underline{\mathbf{1}}_{AA} & -\underline{\mathbf{H}}_{AB}\left(\underline{\mathbf{H}}_{BB} - \underline{\mathbf{1}}_{BB}E\right)^{-1} \\ \underline{\mathbf{0}}_{BA} & \underline{\mathbf{1}}_{BB} \end{bmatrix} \tag{3}$$

we may left-multiply Eq. (2) by it to obtain:

$$\begin{bmatrix} \underline{\mathbf{H}}_{AA}^{eff} - \underline{\mathbf{1}}_{AA}E & \underline{\mathbf{0}}_{AB} \\ \underline{\mathbf{0}}_{BA} & \underline{\mathbf{H}}_{BB} - \underline{\mathbf{1}}_{BB}E \end{bmatrix} \begin{bmatrix} \mathbf{v'}_A \\ \mathbf{v'}_B \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \tag{4}$$

$$\begin{bmatrix} \mathbf{v'}_A \\ \mathbf{v'}_B \end{bmatrix} = \begin{bmatrix} \mathbf{v}_A \\ \left(\underline{\mathbf{H}}_{BB} - \underline{\mathbf{1}}_{BB}E\right)^{-1}\mathbf{v}_A + \mathbf{v}_B \end{bmatrix} \tag{5}$$

$$\left(\underline{\mathbf{H}}_{AA}^{eff} - \underline{\mathbf{1}}_{AA}E\right) = \left(\underline{\mathbf{H}}_{AA} - \underline{\mathbf{1}}_{AA}E\right) - \underline{\mathbf{H}}_{AB}\left(\underline{\mathbf{H}}_{BB} - \underline{\mathbf{1}}_{BB}E\right)^{-1}\underline{\mathbf{H}}_{AB}^{\dagger}. \tag{6}$$

The full, linear eigenproblem has thus been replaced by the smaller class-$A$ only nonlinear eigneproblem,

$$\left[\left(\underline{\mathbf{H}}_{AA} - \underline{\mathbf{1}}_{AA}E\right) - \underline{\mathbf{H}}_{AB}\left(\underline{\mathbf{H}}_{BB} - \underline{\mathbf{1}}_{BB}E\right)^{-1}\underline{\mathbf{H}}_{AB}^{\dagger}\right]\mathbf{v}_A = \mathbf{0}_A. \tag{7}$$

The second term in the effective Hamiltonian, Eq. (6) shows explicitly how the effect of the class-$B$ states is reflected in the class-$A$ only eigenproblem. While Eq. (7) is exact, its nonlinearity presents more numerical difficulties in solution than does an equivalently-sized linear eigenproblem. For example, while there is only one physical eigenvalue for each nondegenerate class-$A$ state, the nonlinear problem generally produces additional eigenvalues which are mathematical artifacts. Moreover, postulated Hamiltonians are almost never energy-dependent, whereas due to the $(\underline{\mathbf{H}}_{BB} - \underline{\mathbf{1}}_{BB}E)^{-1}$ term the effective Hamiltonian of Eqs. (6)–(7) most definitely is. Although when the appropriate conditions hold Eq. (7) can be linearized, other energy-independent partitioning methods are more straightforward and useful for implicit effective Hamiltonians.

### 2.3 Energy-independent partitioning: general

The goal of energy-independent partitioning is to find a unitary transformation which reduces the Hamiltonian in the new basis to block-diagonal; the transformation matrix is often written as an exponential in order to exploit the multiple commutator expansion from quantum mechanics [7–9]. We seek a matrix, $\underline{\mathbf{S}}$, to block-diagonalize the Hamiltonian:

$$\underline{\mathbf{H}}' = e^{-\underline{\mathbf{S}}}\underline{\mathbf{H}}e^{\underline{\mathbf{S}}} \tag{8}$$

$$\underline{\mathbf{H}}' = \begin{bmatrix} \underline{\mathbf{H}}'_{AA} & \underline{\mathbf{0}}_{AB} \\ \underline{\mathbf{0}}_{BA} & \underline{\mathbf{H}}'_{BB} \end{bmatrix}, \quad \underline{\mathbf{H}} = \begin{bmatrix} \underline{\mathbf{H}}_{AA} & \underline{\mathbf{H}}_{AB} \\ \underline{\mathbf{H}}_{AB}^{\dagger} & \underline{\mathbf{H}}_{BB} \end{bmatrix}. \tag{9}$$

For the transformation to be unitary, the matrix $\underline{\mathbf{S}}$ must be anti-Hermitian:

$$\left(\exp\left(\underline{\mathbf{S}}\right)\right)^{\dagger} = \exp\left(\underline{\mathbf{S}}^{\dagger}\right) = \exp\left(-\underline{\mathbf{S}}\right) \Rightarrow \underline{\mathbf{S}}^{\dagger} = -\underline{\mathbf{S}}, \tag{10}$$

so that $\underline{\mathbf{S}}$ can take the form:

$$\underline{\mathbf{S}} = \begin{bmatrix} \underline{\mathbf{0}}_{AA} & \underline{\mathbf{M}} \\ -\underline{\mathbf{M}}^{\dagger} & \underline{\mathbf{0}}_{BB} \end{bmatrix}. \tag{11}$$

We may solve for the $N_A \times N_B$ matrix $\underline{\mathbf{M}}$ (or equivalently, $\underline{\mathbf{S}}$), by expanding Eq. (8) using the multiple-commutator formula [11]:

$$\underline{\mathbf{H}}' = \underline{\mathbf{H}} + \left[\underline{\mathbf{H}}, \underline{\mathbf{S}}\right] + \frac{1}{2!}\left[\left[\underline{\mathbf{H}}, \underline{\mathbf{S}}\right], \underline{\mathbf{S}}\right] + \ldots \tag{12}$$

Interestingly, similar expansion formulas may be found in mathematical journals from over a century ago [12,13]. From Eq. (12) it is clear that the matrix $\underline{\mathbf{M}}$ will be obtained perturbatively. The idea is to require the off-diagonal blocks of $\underline{\mathbf{H}}'$ to be zero up to a desired order in $\underline{\mathbf{M}}$. The first-order solution is straightforward:

$$\begin{aligned}
&\begin{bmatrix} \underline{\mathbf{H}}'_{AA} & \underline{\mathbf{0}}_{AB} \\ \underline{\mathbf{0}}_{BA} & \underline{\mathbf{H}}'_{BB} \end{bmatrix} = \begin{bmatrix} \underline{\mathbf{H}}_{AA} & \underline{\mathbf{H}}_{AB} \\ \underline{\mathbf{H}}^{\dagger}_{AB} & \underline{\mathbf{H}}_{BB} \end{bmatrix} \\
&\quad + \begin{bmatrix} -\underline{\mathbf{H}}_{AB}\underline{\mathbf{M}}^{\dagger} - \underline{\mathbf{M}}\underline{\mathbf{H}}^{\dagger}_{AB} & \underline{\mathbf{H}}_{AA}\underline{\mathbf{M}} - \underline{\mathbf{M}}\underline{\mathbf{H}}_{BB} \\ -\underline{\mathbf{H}}_{BB}\underline{\mathbf{M}}^{\dagger} + \underline{\mathbf{M}}^{\dagger}\underline{\mathbf{H}}_{AA} & \underline{\mathbf{H}}^{\dagger}_{AB}\underline{\mathbf{M}} + \underline{\mathbf{M}}^{\dagger}\underline{\mathbf{H}}_{AB} \end{bmatrix} + O\left(\underline{\mathbf{M}}^2\right) \qquad (13) \\
&\Rightarrow \underline{\mathbf{0}}_{AB} = \underline{\mathbf{H}}_{AB} + \underline{\mathbf{H}}_{AA}\underline{\mathbf{M}} - \underline{\mathbf{M}}\underline{\mathbf{H}}_{BB}. \qquad (14)
\end{aligned}$$

There are several ways to solve Eq. (14). In the most general case, one constructs a further infinite perturbation series for $\underline{\mathbf{M}}$, assuming that $\underline{\mathbf{H}}_{BB}$ is nonsingular [7,9]:

$$\underline{\mathbf{M}} = \underline{\mathbf{H}}_{AB}\underline{\mathbf{H}}^{-1}_{BB} + \underline{\mathbf{H}}_{AA}\underline{\mathbf{M}}\underline{\mathbf{H}}^{-1}_{BB}. \qquad (15)$$

Equation (15) is general but it has some significant difficulties. First, note that when solving for $\underline{\mathbf{M}}$ in this way, $\underline{\mathbf{M}}$ contains terms to all orders in the coupling matrix $\underline{\mathbf{H}}_{AB}$. Second, and perhaps more importantly, while Eq. (14) is obviously invariant under a real diagonal shift, $\nu$,

$$\begin{aligned}
\underline{\mathbf{0}}_{AB} &= \underline{\mathbf{H}}_{AB} + \left(\underline{\mathbf{H}}_{AA} - \underline{\mathbf{1}}_{AA}\nu\right)\underline{\mathbf{M}} - \underline{\mathbf{M}}\left(\underline{\mathbf{H}}_{BB} - \underline{\mathbf{1}}_{BB}\nu\right) \\
&= \underline{\mathbf{H}}_{AB} + \underline{\mathbf{H}}_{AA}\underline{\mathbf{M}} - \underline{\mathbf{M}}\underline{\mathbf{H}}_{BB}, \qquad (16)
\end{aligned}$$

Equation (15) clearly is not. The only way to preserve invariance under such a shift when using Eq. (15) is to solve for $\underline{\mathbf{M}}$ to all orders by solving the analog of Eq. (15) for each multiple commutator in Eq. (12). An alternate method is therefore desirable.

### 2.4 Energy-independent partitioning: diagonal block eigenbasis

The problem of invariance under an arbitrary shift can be addressed by breaking $\underline{\mathbf{H}}_{AA}$ and $\underline{\mathbf{H}}_{BB}$ up into diagonal parts $\left(\underline{\mathbf{H}}^{(d)}_{AA}, \underline{\mathbf{H}}^{(d)}_{BB}\right)$ and off-diagonal parts $\left(\underline{\mathbf{V}}_{AA}, \underline{\mathbf{V}}_{BB}\right)$: $\underline{\mathbf{H}}_{AA} = \underline{\mathbf{H}}^{(d)}_{AA} + \underline{\mathbf{V}}_{AA}$, $\underline{\mathbf{H}}_{BB} = \underline{\mathbf{H}}^{(d)}_{BB} + \underline{\mathbf{V}}_{BB}$ and this approach has been used [8]. However, doing so still requires solving an infinite perturbation series for the matrix, $\underline{\mathbf{M}}$. A much better approach is to use a basis which fully diagonalizes $\underline{\mathbf{H}}_{AA}$ and $\underline{\mathbf{H}}_{BB}$:

$$\begin{bmatrix} \underline{\mathbf{H}}_{AA} & \underline{\mathbf{0}}_{AB} \\ \underline{\mathbf{0}}_{BA} & \underline{\mathbf{H}}_{BB} \end{bmatrix} \begin{bmatrix} \mathbf{v}^{(\alpha)}_{A} \\ \mathbf{0}_{B} \end{bmatrix} = \varepsilon^{(A)}_{\alpha} \begin{bmatrix} \mathbf{v}^{(\alpha)}_{A} \\ \mathbf{0}_{B} \end{bmatrix}; \quad \begin{bmatrix} \underline{\mathbf{H}}_{AA} & \underline{\mathbf{0}}_{AB} \\ \underline{\mathbf{0}}_{BA} & \underline{\mathbf{H}}_{BB} \end{bmatrix} \begin{bmatrix} \mathbf{0}_{A} \\ \mathbf{v}^{(\beta)}_{B} \end{bmatrix} = \varepsilon^{(B)}_{\beta} \begin{bmatrix} \mathbf{0}_{A} \\ \mathbf{v}^{(\beta)}_{B} \end{bmatrix}. \qquad (17)$$

In this basis $\underline{\mathbf{H}}_{AA}$ and $\underline{\mathbf{H}}_{BB}$ are diagonal:

$$\left[\underline{\mathbf{H}}_{AA}\right]_{\alpha,\alpha'} = \varepsilon^{(A)}_{\alpha}\delta_{\alpha,\alpha'}, \quad \left[\underline{\mathbf{H}}_{BB}\right]_{\beta,\beta'} = \varepsilon^{(B)}_{\beta}\delta_{\beta,\beta'}. \qquad (18)$$

The products of these matrices with the as-yet unknown matrix, $\underline{\mathbf{M}}$, are thus easily found:

$$\left[\underline{\mathbf{H}}_{AA}\underline{\mathbf{M}}\right]_{\alpha,\beta} = \sum_{\eta=1}^{N_A} \left[\underline{\mathbf{H}}_{AA}\right]_{\alpha,\eta} \left[\underline{\mathbf{M}}\right]_{\eta,\beta} = \varepsilon_{\alpha}^{(A)} \left[\underline{\mathbf{M}}\right]_{\alpha,\beta} \tag{19}$$

$$\left[\underline{\mathbf{M}}\underline{\mathbf{H}}_{BB}\right]_{\alpha,\beta} = \sum_{\gamma=1}^{N_B} \left[\underline{\mathbf{M}}\right]_{\alpha,\gamma} \left[\underline{\mathbf{H}}_{BB}\right]_{\gamma,\beta} = \varepsilon_{\beta}^{(B)} \left[\underline{\mathbf{M}}\right]_{\alpha,\beta}. \tag{20}$$

Substituting Eqs. (19) and (20) into Eq. (14) yields a particularly satisfying, closed-form solution for the first-order part of the matrix $\underline{\mathbf{M}}$, denoted $\underline{\mathbf{M}}^{(1)}$:

$$\left[\underline{\mathbf{M}}^{(1)}\right]_{\alpha,\beta} = \frac{1}{\varepsilon_{\beta}^{(B)} - \varepsilon_{\alpha}^{(A)}} \left[\underline{\mathbf{H}}_{AB}\right]_{\alpha,\beta}. \tag{21}$$

In Eq. (21) we assume that $\varepsilon_{\beta}^{(B)} \neq \varepsilon_{\alpha}^{(A)}$, which is always satisfied if the class-$A$ and class-$B$ states are sufficiently separated in energy. If they are not well-separated then a small $\underline{\mathbf{H}}_{AB}$ can strongly couple them, making a perturbation expansion unsuitable, just as in the usual quantum-mechanical perturbation theory. However, when the two classes are well-separated, observe that the full first-order content of $\underline{\mathbf{M}}$ has been found, and that there is no infinite series to truncate. Keeping track of the order in the perturbation theory is therefore considerably easier. As will be shown below, higher-order terms in $\underline{\mathbf{M}}$ from multiple commutators will not change the first-order contribution, Eq. (21), and will turn out to be of odd order in $\underline{\mathbf{H}}_{AB}$.

The final objective of Eq. (14) is, of course, to find the matrix $\underline{\mathbf{H}'}_{AA}$ to a desired order in the coupling, $\underline{\mathbf{H}}_{AB}$. Corrections up to second order are included in the first three terms of Eq. (12). Equation (13) has the single commutator; the double commutator is straightforward if slightly tedious. Its contribution to the $AA$ block is:

$$\frac{1}{2}\left[\left[\underline{\mathbf{H}}, \underline{\mathbf{S}}\right], \underline{\mathbf{S}}\right]_{AA} = \underline{\mathbf{M}}\underline{\mathbf{H}}_{BB}\underline{\mathbf{M}}^{\dagger} - \frac{1}{2}\left\{\underline{\mathbf{H}}_{AA}, \underline{\mathbf{M}}\underline{\mathbf{M}}^{\dagger}\right\}. \tag{22}$$

Combining Eqs. (22) and (13) then,

$$\underline{\mathbf{H}'}_{AA} \approx \underline{\mathbf{H}}_{AA} - \underline{\mathbf{H}}_{AB}\underline{\mathbf{M}}^{\dagger} - \underline{\mathbf{M}}\underline{\mathbf{H}}_{AB}^{\dagger} + \underline{\mathbf{M}}\underline{\mathbf{H}}_{BB}\underline{\mathbf{M}}^{\dagger} - \frac{1}{2}\left\{\underline{\mathbf{H}}_{AA}, \underline{\mathbf{M}}\underline{\mathbf{M}}^{\dagger}\right\}. \tag{23}$$

The matrix products in Eq. (23), although somewhat numerous, are relatively simple to compute due to the forms taken by the matrices involved. Substituting Eqs. (18) and (21) into Eq. (23) gives a surprisingly compact expression for the elements of the effective class-$A$ Hamiltonian:

$$\left[\underline{\mathbf{H}'}_{AA}\right]_{\alpha,\alpha'} \approx \varepsilon_{\alpha}^{(A)}\delta_{\alpha,\alpha'} - \frac{1}{2}\sum_{\gamma=1}^{N_B}\left[\frac{1}{\varepsilon_{\gamma}^{(B)} - \varepsilon_{\alpha}^{(A)}} + \frac{1}{\varepsilon_{\gamma}^{(B)} - \varepsilon_{\alpha'}^{(A)}}\right]\left[\underline{\mathbf{H}}_{AB}\right]_{\alpha,\gamma}\left[\underline{\mathbf{H}}_{AB}\right]_{\alpha',\gamma}^{*} \tag{24}$$

Observe that because the term in square brackets is symmetric in the class-$A$ states $(\alpha, \alpha')$, the effective class-$A$ Hamiltonian, $\underline{\mathbf{H}}'_{AA}$, is clearly Hermitian.

We now show that with this choice of basis, higher-order corrections to $\underline{\mathbf{M}}$ will always be odd-order in $\underline{\mathbf{H}}_{AB}$. The proof follows from writing $\underline{\mathbf{H}}$ as a sum of a block-diagonal part, $\underline{\mathbf{H}}_D$, and a block-off-diagonal part, $\underline{\mathbf{H}}_\Omega$:

$$\underline{\mathbf{H}} = \underline{\mathbf{H}}_D + \underline{\mathbf{H}}_\Omega = \begin{bmatrix} \underline{\mathbf{H}}_{AA} & \underline{\mathbf{0}}_{AB} \\ \underline{\mathbf{0}}_{BA} & \underline{\mathbf{H}}_{BB} \end{bmatrix} + \begin{bmatrix} \underline{\mathbf{0}}_{AA} & \underline{\mathbf{H}}_{AB} \\ \underline{\mathbf{H}}^\dagger_{AB} & \underline{\mathbf{0}}_{BB} \end{bmatrix}. \tag{25}$$

Next, observe that products (right and left) of the block-off-diagonal matrix, $\underline{\mathbf{S}}$, with any block-diagonal matrix, $\underline{\mathbf{D}}$, or block-off-diagonal matrix, $\underline{\mathbf{\Omega}}$,

$$\underline{\mathbf{D}} = \begin{bmatrix} \underline{\mathbf{D}}_{AA} & \underline{\mathbf{0}}_{AB} \\ \underline{\mathbf{0}}_{BA} & \underline{\mathbf{D}}_{BB} \end{bmatrix}; \quad \underline{\mathbf{\Omega}} = \begin{bmatrix} \underline{\mathbf{0}}_{AA} & \underline{\mathbf{\Omega}}_{AB} \\ \underline{\mathbf{\Omega}}^\dagger_{AB} & \underline{\mathbf{0}}_{BB} \end{bmatrix}, \tag{26}$$

are respectively block-off-diagonal or block-diagonal. The matrix $\underline{\mathbf{M}}$ is found by requiring the off-diagonal blocks of Eq. (12) to vanish. Thus corrections to $\underline{\mathbf{M}}$ are found by solving this equation to the desired order and appear in the off-diagonal blocks of the multiple commutators.

Formally, one writes $\underline{\mathbf{M}}$ as a perturbation expansion in orders of $\underline{\mathbf{H}}_{AB}$, with a perturbation parameter to keep track of the order:

$$\underline{\mathbf{M}} = \sum_{n=1}^{\infty} \underline{\mathbf{M}}^{(n)} \tag{27}$$

where $\underline{\mathbf{M}}^{(n)}$ is of order $n$in the matrix $\underline{\mathbf{H}}_{AB}$, and obviously there is no zeroth-order term. Therefore the zero, double, quadruple, etc., commutators of $\underline{\mathbf{S}}$ with $\underline{\mathbf{H}}_\Omega$ are off-diagonal and thus contribute to the expansion of $\underline{\mathbf{M}}$. Because both $\underline{\mathbf{S}}$ and $\underline{\mathbf{H}}_\Omega$are first-order in $\underline{\mathbf{H}}_{AB}$, the order of the contribution is one higher than the number of commutators. Likewise, the single, triple, quintuple, etc. commutators of $\underline{\mathbf{S}}$ with $\underline{\mathbf{H}}_D$ are off-diagonal and also contribute to the expansion of $\underline{\mathbf{M}}$. Here, however, the order the same as the number of commutators because $\underline{\mathbf{H}}_D$ is independent of $\underline{\mathbf{H}}_{AB}$. No terms second order in $\underline{\mathbf{H}}_{AB}$ can come from the commutators of $\underline{\mathbf{S}}$ with $\underline{\mathbf{H}}_\Omega$. Only the single commutator of $\underline{\mathbf{S}}$ with $\underline{\mathbf{H}}_D$ can contribute a second-order term. Hence, $\underline{\mathbf{M}}^{(2)}$ vanishes. This single commutator could also contribute a fourth-order term, but for the double commutator of $\underline{\mathbf{S}}$ with $\underline{\mathbf{H}}_\Omega$ to contribute a fourth order term $\underline{\mathbf{M}}^{(2)}$ cannot vanish. This condition also holds for the triple commutator of $\underline{\mathbf{S}}$ with $\underline{\mathbf{H}}_D$, so $\underline{\mathbf{M}}^{(4)}$ vanishes. One can continue this reasoning to higher orders ad infinitum. One could equally well simply work out corrections starting with the linear term, Eq. (21), obtaining only odd-order corrections. Thus it follows that only odd-order terms $\underline{\mathbf{M}}^{(2m+1)}$ survive in Eq. (27).

In concluding this section we comment on the relationship of the present method to some previous work [7,9,14–16]. As discussed in subsections C and D above, Refs. [7–9] also carry out the decoupling using Eq. (8), however all differ from this work. References [7,9] construct the decoupling matrix, $\underline{\mathbf{M}}$, from the infinite perturbation series, Eq. (15), instead of Eq. (14), and Ref. [8] still includes off-diagonal

parts of $\underline{\mathbf{H}}_{AA}$ and $\underline{\mathbf{H}}_{BB}$ in the perturbation. In contrast the present method fully diagonalizes $\underline{\mathbf{H}}_{AA}$ and $\underline{\mathbf{H}}_{BB}$ so that Eq. (14) can be solved exactly for the first-order part of $\underline{\mathbf{M}}$. The method of Refs. [14,16] requires solving for selected roots of the coupled eigenproblem, Eq. (1): See, in particular, Eqs. (16)–(17) of Ref. [14] and the following discussion. The present method, in contrast, does not require any eigenstates of the coupled problem. The method of Ref. [15] is also closely related, and could be applied to the present problem by taking $\underline{\mathbf{H}}_D$ and $\underline{\mathbf{H}}_\Omega$ of Eq. (25) to be respectively $\hat{H}_0$ and $\hat{V}$. However, as discussed in Sect. 2.5 of Ref. [15] the resulting effective Hamiltonian is non-Hermitian. Conversely, in Eq. (24) here the effective class-$A$ Hamiltonian, $\underline{\mathbf{H}'}_{AA}$, is unambiguously Hermitian.

## 3 Application: spin–orbit splitting in graphene

We now use the Digonal Block Eigenbasis method of Sect. 2.4. above to calculate the spin–orbit splitting in graphene at the $K$-point due to $d$-orbitals. The full model used includes three orbitals per atom: $\{p_z, d_{yz}, d_{zx}\}$ and is detailed in Ref. [17]; in the geometry adopted there the $K$-point occurs at $\mathbf{k}_K = (2\pi/(3a))\left(\mathbf{e}_x + \mathbf{e}_y/\sqrt{3}\right)$. Unlike the $p_z$-orbitals, the $d$-orbitals do have a spin–orbit matrix element between orbitals on the same atom:

$$\langle yz;\uparrow;\mathbf{R}|\,\hat{H}_{so}\,|zx;\uparrow;\mathbf{R}\rangle = i\lambda_d; \quad \langle yz;\downarrow;\mathbf{R}|\,\hat{H}_{so}\,|zx;\downarrow;\mathbf{R}\rangle = -i\lambda_d \tag{28}$$

In Eq. (28) $\mathbf{R}$ is the atom location, the arrows indicate the spin quantum number, and $\lambda_d$ is the (real) spin–orbit parameter. From Eq. (28) it is clear that the up- and down-spin states are not coupled by the spin–orbit interaction. This considerably simplifies the calculation, since we need only solve the spin-up problem: Changing the sign on the spin–orbit parameter in the spin-up result immediately gives the spin-down result. We will use partitioning to decouple the $p_z$- and $d$-orbitals to first order and thereby reflect this spin–orbit interaction onto the effective $p_z$-only model.

In the basis defined in Eq. (3) of Ref. [17] the diagonal blocks of the Hamiltonian matrix are not themselves diagonal. However, changing the basis for the $d$-orbitals to:

$$|d1\rangle = \frac{1}{2}\left[|yz+;\mathbf{k}_K\rangle + i\,|zx-;\mathbf{k}_K\rangle - |yz-;\mathbf{k}_K\rangle - i\,|zx+;\mathbf{k}_K\rangle\right] \tag{29}$$

$$|d2\rangle = \frac{1}{2}\left[|yz+;\mathbf{k}_K\rangle + i\,|zx-;\mathbf{k}_K\rangle + |yz-;\mathbf{k}_K\rangle + i\,|zx+;\mathbf{k}_K\rangle\right] \tag{30}$$

$$|d3\rangle = \frac{1}{2}\left[|yz+;\mathbf{k}_K\rangle - i\,|zx-;\mathbf{k}_K\rangle + |yz-;\mathbf{k}_K\rangle - i\,|zx+;\mathbf{k}_K\rangle\right] \tag{31}$$

$$|d4\rangle = \frac{1}{2}\left[|yz+;\mathbf{k}_K\rangle - i\,|zx-;\mathbf{k}_K\rangle - |yz-;\mathbf{k}_K\rangle + i\,|zx+;\mathbf{k}_K\rangle\right] \tag{32}$$

results in a Hamiltonian matrix with blocks which are themselves nearly diagonal.

$$\underline{\mathbf{H}} = \begin{bmatrix} \underline{\mathbf{H}}_{p,p} & \underline{\mathbf{H}}_{p,d} \\ \underline{\mathbf{H}}_{p,d}^{\dagger} & \underline{\mathbf{H}}_{d,d} \end{bmatrix}; \quad \underline{\mathbf{H}}_{p,p} = \begin{bmatrix} E_p & 0 \\ 0 & E_p \end{bmatrix} \tag{33}$$

$$\underline{\mathbf{H}}_{d,d} = \begin{bmatrix} E_d + \lambda_d & 0 & 0 & 0 \\ 0 & E_d - \lambda_d & 0 & 0 \\ 0 & 0 & E_d + \lambda_d & -2U_{d,d} \\ 0 & 0 & -2U_{d,d} & E_d - \lambda_d \end{bmatrix};$$

$$\underline{\mathbf{H}}_{p,d} = \begin{bmatrix} -iU_{p,d} & -iU_{p,d} & 0 & 0 \\ -iU_{p,d} & iU_{p,d} & 0 & 0 \end{bmatrix}. \tag{34}$$

In Eq. (34), the parameters $U$ are defined in terms of the two-center integrals (Slater–Koster parameters [18]) as:

$$U_{p,d} = \frac{3}{2} V_{pd\pi}; \quad U_{d,d} = \frac{3}{4} \left( V_{dd\pi} - V_{dd\delta} \right) \tag{35}$$

For a good discussion of tight-binding models in general, we refer the reader to the books by Harrison [19,20].

Observe from $\underline{\mathbf{H}}_{p,d}$ in Eq. (34) that $\underline{\mathbf{H}}_{p,p}$ is not at all coupled to the lower diagonal block of $\underline{\mathbf{H}}_{d,d}$, the $\{|d3\rangle, \ |d4\rangle\}$ states. Consequently, it is not necessary to diagonalize this block: Its eigenstates play no role in the effective $p$–$p$ Hamiltonian, $\underline{\mathbf{H}}'_{p,p}$. At this point obtaining $\underline{\mathbf{H}}'_{p,p}$ involves merely substituting the matrix elements in Eqs. (33)–(34) into Eq. (24). The result is:

$$\underline{\mathbf{H}}'_{p,p} = \begin{bmatrix} E_p + h_+ & h_- \\ h_- & E_p + h_+ \end{bmatrix}; \quad h_\pm = -U_{p,d}^2 \left[ \frac{1}{E_d + \lambda_d - E_p} \pm \frac{1}{E_d - \lambda_d - E_p} \right] \tag{36}$$

The effective Hamiltonian in Eq. (36) is easily diagonalized, resulting in eigenvalues:

$$E'_{p,\pm} = E_p - \frac{2U_{p,d}^2}{E_d \pm \lambda_d - E_p}. \tag{37}$$

The splitting at the $K$-point is the magnitude of the difference in eigenvalues:

$$\Delta E_K = \left| E'_{p,-} - E'_{p,+} \right| = \frac{4U_{p,d}^2 \lambda_d}{\left( E_d - E_p \right)^2 - \lambda_d^2} \approx \frac{9V_{pd\pi}^2 \lambda_d}{\left( E_d - E_p \right)^2}, \quad |\lambda_d| \ll \left| E_d - E_p \right|. \tag{38}$$

In Eq. (38) we used Eq. (35) and the last approximation is the expression obtained in Ref. [9], employing a perturbation series based on Eq. (15) after first taking $E_p$ as a reference. Note that in the full expression for the splitting no assumption was made on the relative magnitude of the $d$-orbital spin–orbit energy. The only assumptions were that the $p$–$d$ coupling is small and that the $p$- and $d$-states are well-separated, which

are common to all perturbation approaches for decoupling the $d$-orbitals from the $p$-orbitals. In the Diagonal Block Eigenbasis method here, this means that the lowest $d$-state at $E_d - \lambda_d$, must be well-separated from the $p$-states at $E_p$. A reasonable criterion is: $E_d - E_p - \lambda_d \geq \left(E_d - E_p\right)/2 \Rightarrow \left(E_d - E_p\right)/2 \geq \lambda_d$.

While the approximation in Eq. (38) is valid in case of graphene studied in Ref. [9], its validity becomes questionable for two-dimensional topological insulator models, also on the hexagonal lattice. The difference in the two energy-independent partitioning methods for a general monoatomic hexagonal lattice can be seen by graphing the ratios of the splittings:

$$\Delta E_K^{Conv} = \frac{9V_{pd\pi}^2 \lambda_d}{\left(E_d - E_p\right)^2} \tag{39}$$

$$\Delta E_K^{Diag} = \frac{9V_{pd\pi}^2 \lambda_d}{\left(E_d - E_p\right)^2 - \lambda_d^2} \tag{40}$$

over a range of $\lambda_d$. As noted above Eq. (39) is the conventional method [9] while Eq. (40) is the Diagonal Block Eigenbasis method here. The range of $\lambda_d$ over which the method is accurate is roughly $0 < \lambda_d \leq \left(E_d - E_p\right)/2$ as mentioned above. The ratio is conveniently written in terms of a scaled spin–orbit parameter, $x$, as

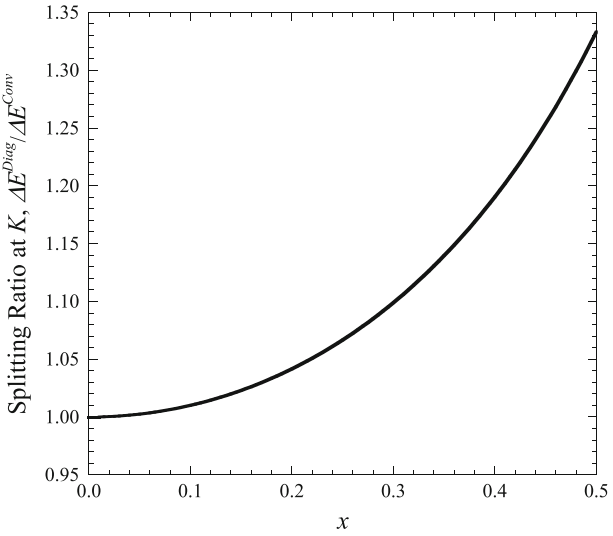


**Fig. 1** Graph of the ratio of spin–orbit splitting at $K$ for a monoatomic hexagonal lattice, as calculated with the Diagonal Block Eigenbasis partitioning to that as calculated with the conventional energy-independent partitioning, $\Delta E_K^{Diag}/\Delta E_K^{conv}$ as a function of the scaled spin–orbit parameter $x = \lambda_d/\left(E_d - E_p\right)$. See Eq. (41). For small spin–orbit coupling the two methods are essentially the same (ratio 1.0), however for $x > 0.3$ the difference becomes more significant, reaching 33 % (ratio 1.33) at $x = 0.5$

$$\frac{\Delta E_K^{Diag}}{\Delta E_K^{conv}} = \frac{1}{1-x^2}; \quad x = \frac{\lambda_d}{E_d - E_p}. \tag{41}$$

The graph of Eq. (41) is shown in Fig. 1. As expected for small values of the spin–orbit interaction (such as in graphene) the two approaches agree very well. For $x > 0.3$, however, the difference from unity becomes steadily more significant, reaching 33 % at $x = 0.5$. Thus the Diagonal Block Eigenbasis method should be more accurate for materials with large spin–orbit interactions.

## 4 Conclusions

Models of physical systems based on effective interactions can be very useful due to their reduced size, but the models themselves can often have counterintuitive properties which result from the effects of eliminated states on the retained, but altered states. We have discussed both energy-dependent and energy-independent effective models, with an emphasis on energy-independent methods for block diagonalizing the Hamiltonian matrix. We have shown that if the eigenbasis of the full diagonal Hamiltonian blocks is used, the transformation matrix takes a particularly simple form to first order in the coupling matrix, and that higher-order corrections are all odd-order. This approach makes keeping track of the order in perturbation theory considerably simpler. We have applied the method to calculate the spin–orbit splitting at the $K$-point in graphene, observing that the constraints on applicability in this approach are much less restrictive than in the conventional method.

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