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## Location of essential spectrum of intermediate Hamiltonians restricted to symmetry subspaces

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A theorem is presented on the location of the essential spectrum of certain intermediate Hamiltonians used to construct lower bounds to bound-state energies of multiparticle atomic and molecular systems. This result is an analog of the Hunziker–Van Winter–Zhislin theorem for exact Hamiltonians, which implies that the continuum of an  $N$ -electron system begins at the ground-state energy for the corresponding system with  $N - 1$  electrons. The work presented here strengthens earlier results of Beattie [SIAM J. Math. Anal. 16, 492 (1985)] in that one may now consider Hamiltonians restricted to the symmetry subspaces appropriate to the permutational symmetry required by the Pauli exclusion principle, or to other physically relevant symmetry subspaces. The associated convergence theory is also given, guaranteeing that all bound-state energies can be approximated from below with arbitrary accuracy.

### I. INTRODUCTION

Variational techniques for obtaining upper bounds to eigenvalues of a multiparticle Hamiltonian  $H$  are well developed and can often yield quite accurate estimates to eigenvalues of interest. However, upper bounds alone cannot provide complete estimates of the error in the approximations to the eigenvalues. To do this one must bracket the eigenvalues of interest by also computing complementary lower bounds.

In general, the computational effort is greater for lower-bound estimation, and the related analysis more subtle, than that required in standard approaches for upper-bound estimation (such as Hartree–Fock and configuration interaction methods). Furthermore, lower-bound procedures usually require some form of additional *a priori* spectral information. For example, Temple's inequality<sup>1,2</sup> can often yield a reasonably tight lower bound to a particular eigenvalue provided that the eigenvalue of interest can be explicitly isolated from the next larger eigenvalue, which requires a good estimate on the next eigenvalue. Such needs for *a priori* spectral information often become problematic in practical circumstance. The method that we consider here, the method of intermediate Hamiltonians, has by contrast fairly relaxed requirements for *a priori* information, though effective use of this information may offer distinct computational challenges.

The method of intermediate Hamiltonians was used with great success by Bazley and Fox<sup>3–6</sup> to obtain lower bounds to He, and by Hill<sup>7</sup> to prove that  $H^-$  has only one bound state. Extensions to three-electron problems proved more difficult, although some results have been obtained.<sup>8–11</sup> This method requires a decomposition of the self-adjoint operator  $H$  as  $H_0 + \hat{H}$ , where information on the discrete spectrum of  $H_0$  is explicitly available and  $\hat{H}$  is a symmetric positive-definite operator (i.e.,  $\hat{H} \geq 0$ ). Those eigenvalues of  $H_0$  that lie below the infimum of the essential spectrum of  $H$  [i.e., the bottom of the continuum, denoted here as  $\lambda_*(H)$ ]

are lower bounds to the corresponding eigenvalues of  $H$ . Because these bounds invariably tend to be quite crude, one seeks improved bounds by carefully approximating  $\hat{H}$  from below (in the sense of quadratic forms). As originally conceived, this was done with an increasing chain of positive semidefinite finite-rank operators. The resulting problem was equivalent to the evaluation of the spectrum of a degenerately perturbed operator with known spectrum.<sup>12</sup> A detailed discussion of intermediate operator methods can be found in Refs. 13–15.

The principal difficulty in applying standard intermediate operator techniques to multiparticle Hamiltonians is that the lowest point of the essential spectrum of the base operator,  $\lambda_*(H_0)$ , often lies below the lowest eigenvalue of  $H$ . Since finite-rank approximations to  $\hat{H}$  produce compact perturbations of  $H_0$  that leave the essential spectrum of  $H_0$  unperturbed, the method as originally developed in Refs. 4 and 5 cannot yield convergent lower bounds. Fox<sup>16</sup> developed a modification of the standard intermediate operator approach utilizing *noncompact* perturbations of the base operator  $H_0$ , yet retaining the critical property of producing computationally resolvable intermediate operators. Recently Beattie<sup>17</sup> showed that a variant of Fox's construction yields intermediate Hamiltonians for which  $\lambda_*(H_0)$  can be made arbitrarily close to  $\lambda_*(H)$ , the lowest point of the essential spectrum of the exact Hamiltonian. This allows, at least in principle, tight lower bounds to all eigenvalues of the Hamiltonian. These results were obtained for the full Hamiltonian operator without considering the permutational symmetries of the system. In calculations for real atomic and molecular systems, one wants to consider Hamiltonians that are restricted to appropriate symmetry subspaces so that the Pauli exclusion principle is satisfied. In this paper we show that the results of Ref. 17 can be extended to such symmetry-restricted Hamiltonians. The crucial point is to extend Beattie's analog of the Hunziker–Van Winter–Zhislin (HVZ)

theorem to intermediate Hamiltonians restricted to appropriate symmetry subspaces.

In addition, we discuss extensions to systems containing several species of identical particles, and to molecular systems. Finally, we show that the lower bounds obtained via this construction converge to the exact eigenvalues of  $H$ . Thus all bound states of  $H$  can, at least in principle, be approximated from below with arbitrary accuracy.

The behavior of a single particle with spin  $s$  is described by a Hamiltonian operator acting on a suitable dense subset of the Hilbert space  $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2s+1}$ . For real electrons, which have two spin states, we have  $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$ . The Hamiltonian for  $N$  identical particles then acts on an appropriate subspace of

$$\mathcal{H}^N = \mathcal{H} \otimes \mathcal{H} \otimes \mathcal{H} \otimes \mathcal{H} \otimes \cdots \otimes \mathcal{H},$$

i.e., the tensor product of  $N$  copies of  $\mathcal{H}$ . If the particles are bosons ( $s = \text{integer}$ ), the  $N$ -particle Hamiltonian must be restricted to the symmetric subspace of  $\mathcal{H}^N$ , which we denote as  $\mathcal{H}_+^N$ . If the particles are fermions ( $s = \text{half-integer}$ ), the  $N$ -particle Hamiltonian must be restricted to the antisymmetric subspace of  $\mathcal{H}^N$ , which we denote as  $\mathcal{H}_-^N$ .

The multiparticle Hamiltonians that we consider have the form

$$H_N = \sum_{i=1}^N [-\Delta_i + W(\mathbf{r}_i)] + \sum_{i < j} V(\mathbf{r}_i - \mathbf{r}_j), \quad (1)$$

where  $\Delta_i$  is the three-dimensional Laplacian acting on coordinates of the  $i$ th particle, and  $W$  and  $V$  are suitable potential functions. The restriction of  $H_N$  to  $\mathcal{H}_+^N$  or  $\mathcal{H}_-^N$  will be denoted  $H_{N,+}$  or  $H_{N,-}$ , respectively. For  $N$  electrons in the field of a fixed nucleus of charge  $Z$ ,  $W(\mathbf{r}) = -Z/r$  and  $V(\mathbf{r}) = 1/r$ , where  $r = |\mathbf{r}|$ . For molecular systems with  $M$  fixed nuclei of charge  $Z_1, \dots, Z_M$  at positions  $\mathbf{R}_1, \dots, \mathbf{R}_M$ ,

$$W(\mathbf{r}) = \sum_{j=1}^M \frac{-Z_j}{|\mathbf{r} - \mathbf{R}_j|} \quad \text{and} \quad V(\mathbf{r}) = \frac{1}{r}.$$

In the molecular case, tractable intermediate Hamiltonians appear to exist only for homonuclear diatomic molecules, in which case the Schrödinger equation for the Hamiltonian

$$h = -\Delta - Z/|\mathbf{r} - \mathbf{R}_1| - Z/|\mathbf{r} - \mathbf{R}_2|$$

can be solved exactly.

We require that the potentials in both the atomic and fixed-nuclei molecular cases satisfy conditions sufficient to assure convergent spectral approximations, as follows:

- (a)  $W$  and  $V \in L^2(\mathbb{R}^3) + [L^\infty(\mathbb{R}^3)]_\epsilon$ ,
- (b)  $V \geq 0$  almost everywhere in  $\mathbb{R}^3$ ,
- (c) the self-adjoint operator corresponding to  $h = -\Delta + W$  is bounded below and has as its spectrum negative eigenvalues of finite multiplicity, and essential spectrum  $[0, \infty)$ .

Although practical applications generally require that  $h$  actually have some negative eigenvalues, the analysis remains valid if some  $h_k$  possesses only essential spectrum  $[0, \infty)$ .

(In the case of diatomic molecules with finite nuclear mass, for example, it might actually be useful to consider

$h_j = -\Delta_j \geq 0$ ; unfortunately, other difficulties prevent us from extending these techniques to molecular systems with finite nuclear mass at present. In the extension to several species of identical particles discussed at the end of Sec. IV, the charge of all particles must have the same sign.)

## II. INTERMEDIATE HAMILTONIANS

Following earlier work, we consider intermediate Hamiltonians that can be expressed in the form

$$H_N^{k\alpha\beta} = \sum_{i=1}^N h_i^{k\alpha} + \sum_{i < j} v_{ij}^\beta, \quad (2)$$

where  $h_i^{k\alpha}$  and  $v_{ij}^\beta$  denote, respectively, approximations to  $h_i = -\Delta_i + W(\mathbf{r}_i)$  and  $V(\mathbf{r}_i - \mathbf{r}_j)$  having the following key properties.

- (i) The approximation  $h_i^{k\alpha}$  has the form  $T_{k\alpha} + \lambda_{k+1}(h)E_k^\perp$ , where  $\lambda_{k+1}(h)$  is the  $k$ th eigenvalue of  $h = -\Delta + W(\mathbf{r})$ ,  $E_k$  is the orthogonal projection onto the span of the eigenspaces corresponding to eigenvalues  $\lambda_1, \dots, \lambda_k$  of  $h$ ,  $E_k^\perp = I - E_k$ ,  $T_{k\alpha}$  is symmetric and has finite rank  $(k + \alpha)$  with range denoted  $\Gamma_{k\alpha}$ , and  $T_{k\alpha} + \lambda_{k+1}(h)E_k^\perp < h$  in the sense of quadratic forms.
- (ii) The approximation  $v_{ij}^\beta$  has finite rank with range  $\Pi_\beta \otimes \Pi_\beta$  for some explicitly known  $\beta$ -dimensional space  $\Pi_\beta \subset \mathcal{H}$ , and  $v_{ij}^\beta < V(\mathbf{r}_i - \mathbf{r}_j)$  in the sense of quadratic forms.

[Although the analysis in Ref. 17 is given for operators on  $L^2(\mathbb{R}^3)$ , it can readily be extended to operators on  $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2s+1}$ . However, we note the following changes in notation:

$$\begin{aligned} n \rightarrow k, \quad A_0^n &\rightarrow hE_k + \lambda_{k+1}(h)E_k^\perp, \\ A_0 &\rightarrow h, \quad \tilde{A}_0^n \rightarrow [h - \lambda_{k+1}(h)]E_k^\perp, \\ \lambda_0^k &\rightarrow \lambda_k(h), \quad A_0^n + \tilde{A}_0^n Q^\alpha \rightarrow T_{k\alpha} + \lambda_{k+1}(h)I, \\ \mathcal{U}_k &\rightarrow E_k \mathcal{H}, \quad \text{Span}_\alpha \{\tilde{A}_0^n q_\nu\} \rightarrow [h - \lambda_{k+1}(h)]E_k^\perp \Omega_\alpha, \\ A_{ij} &\rightarrow V(\mathbf{r}_i - \mathbf{r}_j), \quad A_{ij} P^\beta \rightarrow v_{ij}^\beta, \\ \Pi_\beta &\rightarrow \Pi_\beta, \quad \mathcal{U}_k \vee \text{span}_\alpha \{\tilde{A}_0^n q_\nu\} \rightarrow \Gamma_{k\alpha}. \end{aligned}$$

The construction of  $T_{k\alpha}$  depends on the spectral resolution of  $h$  and the choice of a finite-dimensional subspace  $\Omega_\alpha \subset \mathcal{H}$ :

$$T_{k\alpha} = hE_k + [h - \lambda_{k+1}(h)]E_k^\perp Q^\alpha,$$

where  $Q^\alpha$  is a nonorthogonal projection operator with range  $\Omega_\alpha$  and kernel  $\{[h - \lambda_{k+1}(h)]E_k^\perp \Omega^\alpha\}^\perp$ . The approximation  $v_{ij}^\beta$  is defined similarly as  $V(\mathbf{r}_i - \mathbf{r}_j)R_{ij}^\beta$ , where  $R_{ij}^\beta$  is a nonorthogonal projection with range  $\Lambda_{ij}^\beta$  and kernel

$\{V(\mathbf{r}_i - \mathbf{r}_j) \Lambda_{ij}^\beta\}^\perp$ . A more complete description and analysis may be found in Refs. 16–18.

Define the subspace  $\mathcal{M}^{k\alpha\beta} = \Gamma_{k\alpha} \vee \Pi_\beta$ . Notice that for a simple two-particle intermediate Hamiltonian given by  $H_2^{k\alpha\beta} = h_i^{k\alpha} + h_j^{k\alpha} + v_{ij}^\beta$ , a full set of explicit reducing spaces may be constructed as  $\mathcal{M}^{k\alpha\beta} \otimes \mathcal{M}^{k\alpha\beta}$ ,  $\mathcal{M}^{k\alpha\beta} \otimes [\mathcal{M}^{k\alpha\beta}]^\perp$ ,  $[\mathcal{M}^{k\alpha\beta}]^\perp \otimes \mathcal{M}^{k\alpha\beta}$ , and  $[\mathcal{M}^{k\alpha\beta}]^\perp \otimes [\mathcal{M}^{k\alpha\beta}]^\perp$ . It is not hard to see that on the last subspace,  $H_2^{k\alpha\beta}$  reduces to a scalar multiple of the identity  $I$ , while on the first subspace it is essentially a matrix operator. On the remaining two subspaces,  $H_2^{k\alpha\beta}$  is effectively a direct product of a matrix operator and a scalar multiple of  $I$ . This means that the spectrum of  $H_2^{k\alpha\beta}$  can be computed explicitly through a matrix diagonalization. However, these subspaces will not be reducing subspaces for  $H_{2,\pm}^{k\alpha\beta}$ . To obtain reducing subspaces with the correct permutational symmetry, the first and last subspaces above must be replaced by their symmetric or antisymmetric components, while the middle two spaces must be replaced by

$$\mathcal{H}_{2,1,\pm}^{k\alpha\beta} = \mathcal{M}^{k\alpha\beta} \otimes [\mathcal{M}^{k\alpha\beta}]^\perp \pm [\mathcal{M}^{k\alpha\beta}]^\perp \otimes \mathcal{M}^{k\alpha\beta}.$$

The construction of reducing subspaces in the  $N$ -particle case follows a similar pattern. To construct reducing subspaces for  $H_{N,\pm}^{k\alpha\beta}$  we let

$$\mathcal{W}_{\xi_1, \dots, \xi_r}^{k\alpha\beta} = \mathcal{N}_1 \otimes \mathcal{N}_2 \otimes \dots \otimes \mathcal{N}_N \quad (3)$$

describe a subspace of  $\mathcal{H}^N$  with

$$\mathcal{N}_i = \mathcal{M}^{k\alpha\beta}, \quad \text{if } i \in \{\xi_1, \dots, \xi_r\},$$

and

$$\mathcal{N}_i = [\mathcal{M}^{k\alpha\beta}]^\perp, \quad \text{if } i \notin \{\xi_1, \dots, \xi_r\}.$$

If permutational symmetry is not considered, then  $\mathcal{W}_{\xi_1, \dots, \xi_r}^{k\alpha\beta}$  will be a reducing subspace for  $H_N^{k\alpha\beta}$ . However,  $\mathcal{W}_{\xi_1, \dots, \xi_r}^{k\alpha\beta}$  will not be a reducing subspace for the symmetry-restricted intermediate Hamiltonians  $H_{N,\pm}^{k\alpha\beta}$ . Therefore we now define

$$\mathcal{H}_{N,r}^{k\alpha\beta} = \bigoplus_{\xi_1, \dots, \xi_r} \mathcal{W}_{\xi_1, \dots, \xi_r}^{k\alpha\beta},$$

i.e.,  $\mathcal{H}_{N,r}^{k\alpha\beta}$  is the span of the unions of all subspaces of the form (3) with exactly  $r$  copies of  $\mathcal{M}^{k\alpha\beta}$  and  $N - r$  copies of  $[\mathcal{M}^{k\alpha\beta}]^\perp$ . Let  $\mathcal{H}_{N,r,\pm}^{k\alpha\beta}$  denote the symmetric and antisymmetric subspaces of  $\mathcal{H}_{N,r}^{k\alpha\beta}$ . Then  $\mathcal{H}_{N,r,\pm}^{k\alpha\beta}$  is a reducing subspace for  $H_{N,\pm}^{k\alpha\beta}$  for all  $r$ , and

$$\mathcal{H}_{\pm}^N = \bigoplus_{r=0}^N \mathcal{H}_{N,r,\pm}^{k\alpha\beta}. \quad (4)$$

### III. LOCATION OF ESSENTIAL SPECTRUM

Let  $\lambda_*(A) = \inf \sigma_{\text{ess}}(A)$  and  $\lambda_1(A) = \inf \sigma(A)$ . For Hamiltonians of the form (1), the celebrated HVZ theorem<sup>19</sup> is equivalent to the statement

$$\lambda_*(H_N) = \lambda_1(H_{N-1}),$$

i.e., the essential spectrum of the Hamiltonian of  $N$  particles in the field of a fixed nucleus (or several fixed nuclei) begins at the lowest eigenvalue of the corresponding system with  $N - 1$  particles. In the case of symmetry-restricted Hamiltonians,  $H_{N,\pm}$ , this result becomes

$$\lambda_*(H_{N,\pm}) = \lambda_1(H_{N-1,\pm}).$$

Beattie<sup>17</sup> gave an analogous formula for intermediate Hamiltonians without symmetry restrictions. The extension of Beattie's formula to symmetry-restricted intermediate Hamiltonians is the following theorem.

**Theorem 1:**  $\lambda_*(H_{N,\pm}^{k\alpha\beta}) = \lambda_1(H_{N-1,\pm}^{k\alpha\beta}) + \lambda_{k+1}(h)$ .

Before proving this result, it will be useful to make some observations about the spectral properties of  $H_{N,r,\pm}^{k\alpha\beta}$ , by which we denote the restriction of  $H_N^{k\alpha\beta}$  to  $\mathcal{H}_{N,r,\pm}^{k\alpha\beta}$ . All eigenfunctions of  $H_{N,r,\pm}^{k\alpha\beta}$  have the form

$$\wp_\pm \{G(x_1, \dots, x_r) g_1(x_{r+1}) \dots g_{N-r}(x_N)\}, \quad (5)$$

where  $x_i = (\mathbf{r}_i, s_i)$  represents the space and spin coordinates of the  $i$ th particle,  $G$  is an eigenfunction of  $H_{r,r}^{k\alpha\beta}$ , the  $g_i$  are in  $[\mathcal{M}^{k\alpha\beta}]^\perp$ , and  $\wp_\pm$  projects onto  $\mathcal{H}_{\pm}^N$ . Thus  $H_{N,r,\pm}^{k\alpha\beta}$  has pure point spectrum consisting of eigenvalues of the form

$$\text{e-val}(H_{N,r,\pm}^{k\alpha\beta}) = \text{e-val}(H_{r,\pm}^{k\alpha\beta}) + (N - r)\lambda_{k+1}(h). \quad (6)$$

However, because  $h^{k\alpha}$  is a multiple of the identity on the infinite-dimensional space  $[\mathcal{M}^{k\alpha\beta}]^\perp$ , the eigenvalues of  $H_{N,r,\pm}^{k\alpha\beta}$  have (i) finite multiplicity, if  $r = N$ ; and (ii) infinite multiplicity, if  $r < N$ . Thus  $H_{N,N,\pm}^{k\alpha\beta}$  has only discrete spectrum, while  $H_{N,r,\pm}^{k\alpha\beta}$  has only essential spectrum when  $N > r$ .

To prove Theorem 1, we first note that (4) implies

$$\lambda_1(H_{n,\pm}^{k\alpha\beta}) = \min_{r=0, \dots, n} \lambda_1(H_{n,r,\pm}^{k\alpha\beta}). \quad (7)$$

Applying a similar analysis to  $\lambda_*(H_{N,\pm}^{k\alpha\beta})$  and using (7) along with the observations above, we find that

$$\begin{aligned} \lambda_*(H_{N,\pm}^{k\alpha\beta}) &= \min_{r=0, \dots, N} \lambda_*(H_{N,r,\pm}^{k\alpha\beta}) \\ &= \min_{r=0, \dots, N-1} \lambda_*(H_{N,r,\pm}^{k\alpha\beta}) \\ &= \min_{r=0, \dots, N-1} \{\lambda_1(H_{r,\pm}^{k\alpha\beta}) \\ &\quad + (N - r)\lambda_{k+1}(h)\} \\ &= \min_{r=0, \dots, N-1} \{\lambda_1(H_{r,\pm}^{k\alpha\beta}) \\ &\quad + [(N - 1) - r]\lambda_{k+1}(h)\} + \lambda_{k+1}(h) \\ &= \min_{r=0, \dots, N-1} \{\lambda_1(H_{N-1,r,\pm}^{k\alpha\beta})\} + \lambda_{k+1}(h) \\ &= \lambda_1(H_{N-1,\pm}^{k\alpha\beta}) + \lambda_{k+1}(h). \end{aligned}$$

### IV. EXTENSION TO SYMMETRY SUBSPACES

Our analysis thus far has not explicitly considered spin. The spin was present implicitly by the inclusion of  $\mathbb{C}^{2s+1}$  in  $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2s+1}$ . When spin is explicitly considered, it suffices to use trial functions  $\Psi$  in  $\mathcal{H}_{\pm}^N$  that have the form

$$\Psi = \sum_{i=1}^r \Phi_i(r_1, \dots, r_N) \phi_i(s_1, \dots, s_N), \quad (8)$$

where  $\Phi_i \in [L^2(\mathbb{R}^3)]^N$  and  $\phi_i \in [\mathbb{C}^{2s+1}]^N$ , and for which  $\{\Phi_i\}$  and  $\{\phi_i\}$  are bases of irreducible representations of the symmetric group  $S_N$ . It is then natural to ask if Theorem 1 can be extended to this situation, i.e., to  $H_{N,\sigma}$  defined as the operator  $H_N$  restricted to the subspace of  $[L^2(\mathbb{R}^3)]^N$  corresponding to the irreducible representation  $\sigma$  of  $S_N$ . Before showing that such an extension is possible, we point out that Theorem 1 actually suffices for most practical calculations. If one is interested in bound states belonging to a particular subspace  $\sigma$ , Theorem 1 implies that it suffices to consider

intermediate Hamiltonians restricted to the subspace  $\mathcal{H}_\sigma^{\rho N}$ , provided that the eigenvalues of interest lie below  $\lambda_*(H_{N,\pm})$ . However, the extension to other irreducible representations, which we give here, is useful for several reasons.

(a) One is occasionally interested in bound states embedded in the continuum, i.e., in energies  $E_\sigma$ , which lie in the region  $\lambda_*(H_{N,\pm}) < E_\sigma < \lambda_*(H_{N,\sigma})$ . (Hill's proof<sup>9</sup> that  $H^-$  has no bound states in the quartet sector is an example of such a situation.)

(b) A similar analysis can be applied to other physically relevant symmetries besides permutational symmetry.

(c) This analysis can be extended to consider several species of particles, as described below.

(d) The spectrum of  $\mathcal{H}_\sigma^{\rho N}$  is a subset of that for  $\mathcal{H}_\pm^{\rho N}$ . Hence restriction to  $\mathcal{H}_\sigma^{\rho N}$  can reduce the density of eigenvalue clusters and increase the gap between computed eigenvalues, as compared to that when  $\mathcal{H}_\pm^{\rho N}$  is used. This improves both the conditioning and convergence rate of computational algorithms used ultimately to resolve the final matrix eigenvalue problem.<sup>20</sup>

Sigalov and Sigal<sup>21,22</sup> have shown how to extend the HVZ theorem to Hamiltonians restricted to symmetry subspaces. We summarize their analysis for Hamiltonians of the form  $H_{N,\sigma}$ . Let  $\sigma$  and  $\omega$  denote irreducible representations of  $S_N$  and  $S_n$ , respectively, with  $n < N$ , so that  $S_n$  is isomorphic to a subgroup of  $S_N$ . Let  $\omega < \sigma$  indicate that the irreducible representation  $\omega$  is present in the decomposition of  $\sigma$  restricted to  $S_n$ . Sigalov and Sigal<sup>21,22</sup> showed that, in the case of Hamiltonians of type (1),

$$\lambda_*(H_{N,\sigma}) = \min_{\omega < \sigma} \lambda_1(H_{N-1,\omega}). \quad (9)$$

The corresponding generalization to intermediate Hamiltonians is the next theorem.

**Theorem 2:**

$$\lambda_*(H_{N,\sigma}^{k\alpha\beta}) = \min_{\omega < \sigma} \lambda_1(H_{N-1,\omega}^{k\alpha\beta}) + \lambda_{k+1}(h). \quad (10)$$

*Proof:* We first note that eigenfunctions of  $H_{N,\sigma}^{k\alpha\beta}$  have the form

$$\rho_\sigma\{G(x_1, \dots, x_r)g_1(x_{r+1}) \cdots g_{N-r}(x_N)\},$$

where the notation is as in Theorem 1, except that  $\sigma$  denotes the restriction to the subspace  $\mathcal{H}_\sigma^{\rho N}$  corresponding to  $\sigma$ , and  $G$  is an eigenfunction of  $H_{r,r,\omega}^{k\alpha\beta}$  with  $\omega < \sigma$ . The proof of Theorem 1 can then be easily extended to this more general case. We omit the details.

It should be clear that our analysis could easily be extended to symmetry subspaces corresponding to several species of identical particles instead of  $N$  electrons, e.g.,  $N_1$  electrons and  $N_2$  muons with  $N_1 + N_2 = N$ . In this case,  $-\Delta_i$  would be replaced by  $-\Delta_i/m_i$  in (1), where  $m_i$  is the mass of particle  $i$ , and  $H_N$  would act on  $\mathcal{H}_-^{N_1} \otimes \mathcal{H}_-^{N_2}$ .

## V. CONVERGENCE

The question of what conditions on the approximating subspaces  $\Lambda_y^\beta$  and  $\Omega_\alpha$  are sufficient to guarantee convergent estimates has been addressed in more general settings by Beattie,<sup>18</sup> Greenlee,<sup>23</sup> Beattie and Greenlee,<sup>24</sup> and Brown.<sup>25</sup> In our setting, the derived density criteria sufficient to guarantee convergence may be succinctly stated:

$$(1) \lim \Lambda_y^\beta \text{ is dense in } [W^{2,2}(\mathbb{R}^3) \otimes \mathbb{C}^{2s+1}] \otimes [W^{2,2}(\mathbb{R}^3) \otimes \mathbb{C}^{2s+1}], \quad (11)$$

$$(2) \lim \Omega_\alpha \text{ is dense in } W^{2,2}(\mathbb{R}^3) \otimes \mathbb{C}^{2s+1}, \quad (12)$$

where  $W^{2,2}(\mathbb{R}^3)$  denotes the second Sobolev space embedded in  $L^2(\mathbb{R}^3)$ . In particular, these density conditions induce core conditions within every symmetry subspace  $\mathcal{H}_\sigma^{\rho N}$  sufficient to produce convergent spectral estimates for  $H_{N,\sigma}^{k\alpha\beta}$ , provided one additional hypothesis holds. The convergence results cited above all carry the proviso that the lowest point of the essential spectrum of the intermediate operators must move up sufficiently to expose the eigenvalues of  $H_{N,\sigma}$  to convergent estimates. That such movement can be guaranteed for the full unrestricted Hamiltonian operator was shown in Refs. 18 and 24. We show here that this is also the case for Hamiltonians restricted to symmetry subspaces.

**Theorem 3:** Under the density hypotheses (11) and (12), the family of intermediate Hamiltonians  $\{H_{N,\sigma}^{k\alpha\beta}\}_{k\alpha\beta}$  provides convergent lower-bound estimates to the lowest point of the essential spectrum of  $H_{N,\sigma}$ :

$$\lim_{k\alpha\beta} \lambda_*(H_{N,\sigma}^{k\alpha\beta}) = \lambda_*(H_{N,\sigma}). \quad (13)$$

As a consequence, every lower eigenvalue of  $H_{N,\sigma}$  is accessible to convergent estimates, and

$$\lim_{k\alpha\beta} \lambda_i(H_{N,\sigma}^{k\alpha\beta}) = \lambda_i(H_{N,\sigma}), \quad (14)$$

for every  $i$  such that  $\lambda_i(H_{N,\sigma}) < \lambda_*(H_{N,\sigma})$ .

*Proof:* Consider first the case  $N = 2$ . We have from (10)

$$\begin{aligned} \lambda_*(H_{2,\sigma}^{k\alpha\beta}) &= \min_{\omega < \sigma} \lambda_1(H_{1,\omega}^{k\alpha\beta}) + \lambda_{k+1}(h) \\ &= \lambda_1(H_1^{k\alpha\beta}) + \lambda_{k+1}(h) \\ &= \lambda_1(h^{k\alpha}) + \lambda_{k+1}(h) \\ &= \lambda_1(h) + \lambda_{k+1}(h) = \lambda_*(H_{2,\sigma}) + \lambda_{k+1}(h). \end{aligned}$$

Since  $\lambda_{k+1}(h) \rightarrow 0$  as  $k \rightarrow \infty$ , (13) holds for  $N = 2$ , and the density conditions (11) and (12) guarantee that (14) holds as well. Now make an induction hypothesis and suppose that (13) and (14) hold for all  $N < M$ , for some  $M > 1$ . We may then deduce that

$$\begin{aligned} \lim_{k\alpha\beta} \lambda_*(H_{M,\sigma}^{k\alpha\beta}) &= \lim_{k\alpha\beta} \min_{\omega < \sigma} \lambda_1(H_{M-1,\omega}^{k\alpha\beta}) \\ &= \min_{\omega < \sigma} \lim_{k\alpha\beta} \lambda_1(H_{M-1,\omega}^{k\alpha\beta}) \\ &= \min_{\omega < \sigma} \lambda_1(H_{M-1,\omega}) = \lambda_*(H_{M,\sigma}). \end{aligned}$$

Hence (13) holds for  $N = M$ , the density criteria again imply (14) for  $N = M$ , and the induction step is completed.

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