DIRECT INTEGRAL DESCRIPTION OF ANGULON

RYTIS JURŠĖNAS

Abstract. We propose a representation of angulon in which the angulon operator is decomposable relative to the field of Hilbert spaces over the probability measure space, and the probability measure corresponds to the total-number operator of phonons. In this representation we are able to find the system of $N + 1$ equations whose solutions form the eigenspace of the angulon operator, where $1 \leq N < \infty$ is the number of phonon excitations. Using this result we estimate the infimum of the spectrum. In the special case $N = 1$, the lowest energy approximates to the value which is already known in the literature. Our findings indicate that two-phonon excitations ($N = 2$) contribute notably to the energy of a molecule in superfluid $^4$He.

1. Introduction

In this paper the object of interest is the angulon, first introduced in [1] and later developed in [2,3]. Angulon represents a rotational analogue of polaron, actively studied in the context of solid state and atomic settings [4,5]. However, non-commutativity and discrete energy spectrum inherent to quantum rotations renders the angulon physics substantially different compared to any of the polaron models. The concept of angulon considerably simplifies the problems involving an impurity possessing orbital angular momentum immersed into a bath of bosons. Thereby it paves the way for understanding cold molecules rotating inside superfluid helium nanodroplets [6] and ultracold gases [3,7], Rydberg electrons in Bose–Einstein condensates [8,9], electronic excitations coupled to phonons in solids [10], and several other systems.

The angulon operator describes a linear-rotor molecule dressed by the bosonic field. The operator consists of the kinetic energies of a molecule and the bosonic field, as well as the interaction potential. The kinetic energy of a molecule is given by $cJ^2$, where $c > 0$ is the rotational constant and where the vector-valued operator $J$ is called the angular momentum operator of a linear-rotor impurity. The bosonic part of the Hamiltonian for a molecular impurity describes bosons with some dispersion relation (typically $k^2$, where $k \geq 0$) and with contact interactions. Using the Bogoliubov transformation which maps bosonic particles to quasi-particles, called phonons, one transforms the bosonic part to the Hamiltonian that describes phonons with a dispersion relation, say $\omega(k)$. One further expresses the creation/annihilation operators of phonons in the angular momentum basis so that the kinetic energy of the bosonic field is the free Hamiltonian, $\int \omega(k)n(k)dk$, of mass $\omega$. Here $n(k)$ is the sum of occupation numbers corresponding to the $i$th
phonon state; \( \iota \) runs over the set \( I \) of pairs \((\lambda, \rho)\), where \( \lambda \in \mathbb{N}_0 \) is the phonon angular momentum and \( \rho \in I_{\lambda} := \{-\lambda, -\lambda + 1, \ldots, \lambda\} \). The integration is performed over \( \mathbb{R}^+ := [0, \infty) \).

In its original form, the interaction potential is given by

\[
(1.1) \quad 2R \int \sum_{\lambda, \rho} U_{\lambda}(k) Y_{\lambda,-\rho}(\hat{o}) \hat{b}_{\lambda \rho}(k) dk.
\]

The angular momentum dependent coupling \( U_{\lambda}(k) \) signifies the strength of the potential and it depends on the microscopic details of the two-body interaction between the impurity and the bosons [3]; typically, \( U_{\lambda}(k) \equiv 0 \) for \( \lambda > 1 \). The spherical harmonic \( Y_{\lambda}(\hat{o}) \) is parametrized by the spherical angles \( \hat{o} \) of a molecule. The dependence on the molecular orientation gives rise to a nonzero commutator \([J, Y_{\lambda}(\hat{o})]\), which is calculated in a usual way [11,12]. The bosonic creation and annihilation operators, \( \hat{b}_{\lambda}(k) \) and \( \hat{b}_{\lambda}(k)^* \), respectively, are defined as ordinary operator fields in the sense of quadratic forms; the reader may refer to [13], [14, Sec. 5.2], and [15, Sec. X.7] for a classic exposition.

Within the framework of the variational approach applied to the ansatz [1] for the many-body quantum state with single-phonon excitation, the eigenvalue \( E < 0 \) of the angulon operator satisfies a Dyson-like equation

\[
(1.2) \quad E = c L (L + 1) - \Sigma_L(E)
\]

where the so-called self-energy is defined as

\[
(1.3) \quad \Sigma_L(E) := \int \sum_{J,\lambda} \frac{2\lambda + 1}{4\pi} \begin{bmatrix} L & \lambda & J \\ 0 & 0 & 0 \end{bmatrix}^2 \frac{U_{\lambda}(k)^2}{cJ(J + 1) + \omega(k) - E} dk.
\]

and \( \begin{bmatrix} L & \lambda & J \\ 0 & 0 & 0 \end{bmatrix} \) is the Clebsch–Gordan coefficient for the tensor product \([L] \otimes [\lambda]\) of \( SO_3 \)-irreducible representations [24–26]. The eigenvalue \( E = E_L \) is labeled by the total angular momentum \( L \) obtained by reducing the tensor product \([J] \otimes [\lambda]\); the highest weight \( J \in \mathbb{N}_0 \) of the third component of the operator \( J = (J_1, J_2, J_3) \) is referred to as the angular momentum of a linear-rotor impurity. We have that \( E \) is of multiplicity \( 2L + 1 \).

1.1. Problem setting. In order to overcome the problem of adding a large number of angular momenta necessary for the analysis of higher-order phonon excitations, the authors in [2] make a one step further by introducing a rotation operator which is generated by the collective angular momentum operator of the many-body bath. The angular momentum operator has the highest weight \( \Lambda \in \mathbb{N}_0 \) and the total angular momentum \( L \) is obtained by reducing \([J] \otimes [\Lambda]\) in a standard way. The transformation is useful when the rotational constant \( c \to 0 \), since in this regime the transformed angulon operator can be diagonalized. Still, the eigenvalue is calculated by using the variational ansatz based on single-phonon excitations, though on top of the transformed operator.

In this paper we propose a scheme for treating higher-order phonon excitations self-consistently. We do not rely on the limit of a slowly rotating impurity \( (c \to 0) \), nor we need an auxiliary variational ansatz. In fact, we construct a reference Hilbert space so that, to some extent, the ansatz is represented by an element of that space \( (\text{cf. (5.20a)) and [1, Eq. (3)])} \). On the other hand, in our approach the number \( N \in \mathbb{N} \) of phonon excitations is arbitrarily large but finite. The angular momentum \( \Lambda \) is then obtained by reducing the tensor product of \( n \in \{0, 1, \ldots, N\} \)
copies of $SO_3$-irreducible representations $[\lambda]$. The latter requires some angular momentum algebra, but the exposition becomes elegant once we introduce certain symmetrization coefficients. As a result, we come by the system of $N+1$ equations whose solutions form the eigenspace of the angulon operator.

To achieve our goals, we reformulate the definition of the angulon operator, which we now show is equivalent to the original one.

1.2. Description of the model. We construct the angulon operator as a decomposable operator, $A = \int_0^\infty A(k)\mu(dk)$, relative to the field $k \mapsto \mathcal{H}(k)$ of Hilbert spaces over the probability measure space $(\mathbb{R}^+, \mathcal{F}, \mu)$. The reader may refer to [16, Sec. 12], [17, Chap. II.2] for basic definitions. Here and elsewhere, the direct integral is assumed over $\mathbb{R}^+$. The crucial point is that now we are able to put the sum $n(k)$ of occupation numbers aside in a certain sense and yet to considerably simplify the spectral analysis of the angulon operator independently of $n(k)$. Assuming further that $\mu \ll dk$, with the Radon–Nikodym derivative $\phi$ supported on the whole $\mathbb{R}^+ = \mathbb{R}^+ \cup \{\infty\}$, we show that the greatest lower bound of $A$ does not depend on $\phi$, and hence on $k \mapsto n(k)$.

- **Measure v. number operator.** To see the connection between $n(k)$ and $\phi(k)$, let us consider a measurable field $k \mapsto V(k)$ of Hilbert spaces over the probability measure space $(\mathbb{R}^+, \mathcal{F}, \mu)$. Let $\mathcal{K} = \int_0^\infty \mathcal{H}(k)\mu(dk)$ be the direct integral of Hilbert spaces and let $\mathcal{H}(k)$ be the symmetric tensor algebra $S(V(k))$ equipped with an appropriate scalar product. Assume we are given two operators, $\omega$ and $n$, defined by measurable fields $k \mapsto \omega(k)I(k)$ and $k \mapsto n(k)$, respectively. Here $\omega(k)$ is the dispersion relation, as discussed above, $I(k)$ is the identity map in $\mathcal{H}(k)$, and $n(k)$ is the multiplication operator by $n \in \mathbb{N}_0$, provided that $n(k)$ acts on vectors from the $n$-th symmetric tensor power $S^n(V(k))$. Given a unit vector $v(k) \in S^n(V(k))$, the scalar product $\langle v, n\omega v \rangle_{\mathcal{K}}$ in $\mathcal{K}$ reads $n \int \omega(k)\mu(dk)$. Now take $\mu \ll dk$ with the Radon–Nikodym derivative $\phi \in L^1(\mathbb{R}^+)$. Then, the scalar product reads $\int \omega(k)n_\phi(k)dk$ with $n_\phi(k) \equiv \phi(k)n$. We thus have obtained a formal analogue of the free bosonic Hamiltonian of mass $\omega$, but now the sum of phonon modes is given by $n_\phi(k)$ for a.e. $k$. The example suggests that the absolutely continuous (a.c.) probability measure corresponds to the total-number operator of phonons.

- **Coherent v. incoherent phonons.** In our approach the creation and annihilation operators $b_\omega$ and $b_\omega^*$, are decomposable operators relative to the field $k \mapsto \mathcal{H}(k)$, and their commutator is given by

$$[b_\omega(k)^*, b_\omega^*(k)] = \delta_{\omega'}I(k)$$

where $\delta_{\omega'} \equiv \delta_{\lambda\lambda'}\delta_{\rho\rho'}$ is the product of Kronecker symbols. At first glance one could expect from (1.4) that such a formulation of the bosonic field is suitable for the study of coherent phonons only. However, the following argument shows that this is not the case.

Recall that $\mathbb{R}^+$ is the union of Borel sets $\sigma_d \in \mathcal{F}$ defined by $\{k \mid F(k) = d\}$ for $d \in \mathbb{N}_0$ and some $\mu$-simple $F: \mathbb{R}^+ \rightarrow \mathbb{C}$. That is, for every $k \in \sigma_d$, the Hilbert space $\mathcal{H}(k)$ is isomorphic to a separable Hilbert space, say $\mathcal{H}_d$, of dimension $d$. Let $j(k)$ be the isomorphism of $\mathcal{H}(k)$ onto $\mathcal{H}_d$ for $k \in \sigma_d$. To the operator $b_\omega(k)$ in $\mathcal{H}(k)$

1The symbol $b_\omega(k)^*$, rather than $b_\omega(k)$, for denoting the annihilation operator seems to us more natural because, as we shall see, the creation operator $b_\omega(k)$ defines the irreducible tensor operator in the sense of Fano–Racah, while its adjoint $b_\omega(k)^*$ does not. Here we follow the notation of [11, 12].
corresponds the operator \( b_{i,d} := j(k) b_i(k) j(k)^* \) in \( \mathfrak{h}_d \) for every \( k \in \sigma_d \). By (1.4), the operators \( b^*_t,d \) and \( b_{t',d} \) satisfy the commutation relation
\[
[b^*_t,d, b_{t',d}] = \delta_{i,i'} \delta_{d,d'} I_d
\]
where \( I_d := j(k)I(k)j(k)^* \), with \( k \in \sigma_d \), is the identity map in \( \mathfrak{h}_d \). We see that (1.5) and the vanishing commutators
\[
[b_{t,d}, b_{t',d}] = 0, \quad [b^*_t,d, b^*_{t',d}] = 0
\]
together define an infinite-dimensional Heisenberg algebra. Thus we have that both

the creation/annihilation operators defined via the operator-valued distributions (as in (1.1); see also [14, Example 5.2.1]) and the creation/annihilation operators defined as decomposable operators relative to \( k \mapsto \mathfrak{h}(k) \) are the representations of a centrally extended Lie algebra \( \mathfrak{g} = \mathfrak{g} \oplus \mathbb{C}I \), with \( \mathfrak{g} \) a commutative Lie algebra. The commutation relations in \( \mathfrak{g} \) are defined by [1, \( \mathfrak{g} \)] = [\( \mathfrak{g} \), 1] = 0 and \( [x, y] = \langle x, y \rangle \) for \( x, y \in \mathfrak{g} \).

\( \mathfrak{g} \) is a Lie algebra provided that \( [\cdot, \cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g} \) is an alternating bilinear map, and a bilinear form \( \langle \cdot, \cdot \rangle : \mathfrak{g} \times \mathfrak{g} \to \mathbb{C} \) is \( \mathfrak{g} \)-invariant. More on this topic can be found in [19].

Now let \( T \) be a representation of \( \mathfrak{g} \) in \( \mathfrak{h} \). Since \( \mathfrak{h} \) and the Fock space \( \mathfrak{F}(L^2(\mathbb{R}^+)) \) are infinite-dimensional separable Hilbert spaces, there exists an isomorphism \( \chi \) mapping \( \mathfrak{h} \) onto \( \mathfrak{F}(L^2(\mathbb{R}^+)) \), and hence \( T_\lambda(\mathfrak{g}) := \chi T(\mathfrak{g}) \chi^{-1} \) is a representation of \( \mathfrak{g} \) in \( \mathfrak{F}(L^2(\mathbb{R}^+)) \). It is a classical result that, for a suitable choice of the bases, the two equivalent representations \( T(\mathfrak{g}) \) and \( T_\lambda(\mathfrak{g}) \) are given by identical matrices; i.e., \( T(\mathfrak{g}) \) in the basis \( B \) of \( \mathfrak{h} \) has the same matrix as \( T_\lambda(\mathfrak{g}) \) in the basis \( \chi B \) of \( \mathfrak{F}(L^2(\mathbb{R}^+)) \). In this respect, the direct integral description of angulon is equivalent to the original one.

1.3. Main results. We now briefly describe our main results, Theorems 7.1, 8.3.

- Eigenspace. Since the angulon operator \( A \) is defined by a measurable field \( k \mapsto A(k) \) relative to \( k \mapsto \mathfrak{h}(k) \), \( E \) is an eigenvalue of \( A \) iff \( E \) is an eigenvalue of \( A(k) \) for \( \mu \)-a.e. \( k \) (recall e.g. [18, Theorem XIII.85(e)]). In Sec. 6 we show that \( A \) is the orthogonal sum of its parts \( A_L \) acting in reducing subspaces \( \mathfrak{h}_L \subset \mathfrak{h} \). Thus, \( E \) is an eigenvalue of \( A_L(k) \) for \( \mu \)-a.e. \( k \) and some \( L \).

An element \( \psi \) of \( \mathfrak{h}_L \) is a square-integrable vector field \( k \mapsto \psi(k) \), and \( \psi \) is in one-to-one correspondence with its coordinates calculated with respect to the field of orthonormal bases of \( \mathfrak{h}_L(k) \) (Theorem 5.3 and (5.18)). When \( \psi_{LM_L}(k) \), with \( M_L \in \{-L, -L + 1, \ldots, L\} \), is an eigenvector of \( A_L(k) \) belonging to \( E = E_{LM_L} \), the coordinates satisfy the relations as given in Theorem 7.1.

- Greatest lower bound. Assuming that \( \mu(\mathbb{R}^+) = \phi(k)dk \) with \( \supp \phi = \mathbb{R}^+ \), we examine the infimum \( E = E_{LM_L} \) of the spectrum of \( A_L \). We show in Theorem 8.3 that \( E \) solves (1.2) for \( N \) phonon excitations, but with different self-energy \( \Sigma_L(E) \geq 0 \); if however \( \Sigma_L(E) \leq 0 \) then \( E = cL(L + 1) \). In particular, when \( N = 1 \) (Corollary 8.4), \( E \) approximates to (1.2), (1.3). When \( N = 2 \) and \( L = 0 \) (Corollary 8.5), \( E \) solves \( E = -\Sigma_0(E) \), where the self-energy is defined as
\[
\Sigma_0(E) := \int_{\mathbb{R}^+} \sum_{\lambda \lambda'} \frac{2\lambda + 1}{4\pi} \frac{U_{\lambda}(k)^2}{c\lambda(\lambda + 1) + \omega(k) - E - \epsilon_\lambda(E,k)} \, dk
\]
and \( f \) is the Cauchy principal value of the integral over \( \mathbb{R}^+ \). Comparing (1.6) with (1.3) for \( L = 0 \), we see that now the denominator contains an additional \( \epsilon_\lambda(E,k) \),
which is defined as

\begin{equation}
\varepsilon_\lambda(\mathcal{E},k) := \frac{1}{2\pi} (-1)^{\lambda} (2\lambda + 1) U_\lambda(k)^2 \sum_\Lambda c_\Lambda (\Lambda + 1) + 2\omega(k) - \mathcal{E}
\end{equation}

for a.e. \( k \), and the sum runs over even numbers \( \Lambda \in \{0, 2, \ldots, 2\lambda\} \). The lowest energy \( \mathcal{E} \leq 0 \) for a molecule in superfluid \(^4\)He is shown in Fig. 1. If we compared the energy with the curve \( 0_0 \) in [1, Fig. 2(a)] for \( N = 1 \), we would see that adding the two-phonon excitations reflects in a significant increase of the lowest energy.

We would like to point out that \( \mathcal{E} \) might not belong to the numerical range \( \Theta_L \) of \( A_L \). Yet \( \mathcal{E} \) lies at the bottom of the closure \( \overline{\Theta_L} \).

1.4. **Outline of the paper.** Sec. 2 is of preliminary character. Here we sum up basic definitions that we use throughout the paper. In Sec. 3 we give a precise definition of the angulon operator within the framework of the direct integral approach. Our definition relies on the hypothesis that the functions \( k \mapsto \omega(k) \) and \( k \mapsto \sum_\lambda (2\lambda + 1)^{3/2} U_\lambda(k) \) are \( \mu \)-essentially bounded. The hypothesis considerably simplifies the presentation, since in this case the angulon operator is a self-adjoint decomposable operator defined on the domain \( \text{dom} J^2 \otimes \mathfrak{R} \), where \( \text{dom} J^2 \) is the maximal domain of \( J^2 \). In Sec. 4 we show that the angulon operator \( A \) is unitarily equivalent to the \( SO_3 \)-scalar tensor operator \( A' \), and we further identify \( A \) with \( A' \). In Sec. 5.1 we introduce the symmetric coefficients of fractional parentage (SCFPs) and describe their properties. With the help of the SCFPs we construct the field of orthonormal bases that transform under rotations in \( \mathfrak{R}(k) \) as an irreducible tensor operator of rank \( \Lambda \) (Theorem 5.3). Then, reducing the tensor product \( [J] \otimes [\Lambda] \rightarrow [L] \), we find reducing subspaces \( \mathfrak{H}_L \) for the angulon operator (Secs. 5.3
and 6). We study the eigenvalues in Sec. 7. Using Theorem 7.1 we examine the numerical range in Sec. 8, and we summarize our findings in Theorem 8.3 and the subsequent corollaries.

2. Preliminaries and notation

Here and elsewhere, \( V \) is the direct integral \( \int^\oplus V(k)\mu(k) \) of a measurable field \( k \mapsto V(k) \) of Hilbert spaces over the probability measure space \( (\mathbb{R}^+, \mathcal{F}, \mu) \). Measurable fields are assumed to be \( \mu \)-measurable. The integral \( \int^\oplus \) means the integral over \( \mathbb{R}^+ \) unless specified otherwise. The scalar product is indexed by the Hilbert space in which it is defined; e.g. \( \langle \cdot, \cdot \rangle_V \) refers to the scalar product in \( V \). Fix \( (e_i(k))_{i \in I} \) as an orthonormal basis of \( V(k) \); the sequence \( (e_i)_{i \in I} \) of measurable vector fields \( k \mapsto e_i(k) \) is a measurable field of orthonormal bases [17, Proposition II.1.4.1].

Let \( \iota = (\iota_1, \ldots, \iota_n) \in \Gamma^n \). To the basis vector \( e_i(k) := \bigotimes_{i=1}^n e_{\iota_i}(k) \) of the \( n \)th tensor power \( T^n(V(k)) \) corresponds the basis vector \( \hat{e}_i(k) := e_i(k) + I(V(k)) \) of the \( n \)th symmetric tensor power \( S^n(V(k)) \). The ideal \( I(V(k)) \) of the tensor algebra \( T(V(k)) \) is generated by the elements of the form \( w(k) \otimes v(k) - v(k) \otimes w(k) \) with \( w(k), v(k) \in V(k) \). When \( n = 0, \iota = \iota_0 = (\iota_1) \) is empty and \( e_{\iota_0}(k) := 1(k) \in T^0(V(k)) \) is the unit element. For notational convenience, we usually write \( \hat{e}_i(k) \) in the form \( \hat{e}_i(k) = \hat{e}_i(k) \), where the symbol \( \otimes \) alludes to the symmetrized tensor product. With this notation \( \hat{e}_{\iota'}(k) \), with \( \iota' \in \Gamma^n \), implies \( \hat{e}_i(k) \otimes \hat{e}_{\iota'}(k) \), and vice versa. According to [17, Proposition II.1.8.10], the field \( k \mapsto e_i(k) \) is measurable, hence so is the field \( k \mapsto \hat{e}_i(k) \).

The action of the symmetric group \( \mathfrak{S}_n \) on a sequence \( \iota \in \Gamma^n \) of length \( n \) is defined as \( \pi \cdot \iota = (\pi_\iota(1), \ldots, \pi_\iota(n)) \) with \( \pi \in \mathfrak{S}_n \) and \( n \in \mathbb{N} \); when \( n = 0, \pi \cdot \iota_0 = \iota_0 \). We have an important, although obvious, relation \( \hat{e}_{\pi \iota}(k) = \hat{e}_i(k) \).

Assume that \( \hat{e}_{\iota}(k) = \hat{e}_i(k) \in S^n(V(k)) \). The symmetric tensor algebra \( S(V(k)) \) completed with the norm that is induced by the scalar product

\[
\langle \hat{e}_{\iota}(k), \hat{e}_i(k) \rangle_{S^n(k)} := \frac{1}{n!} \sum_{\pi \in \mathfrak{S}_n} \prod_{i=1}^n \langle v_i(k), u_{\pi(i)}(k) \rangle_{V(k)}
\]

is the Hilbert space, denoted by \( \mathcal{H}(k) \) [20, Secs. IV.2.4, V.3]; \( \mathcal{H} = \int^\oplus \mathcal{H}(k)\mu(\mathrm{d}k) \) is the direct integral of a measurable field \( k \mapsto \mathcal{H}(k) \) of Hilbert spaces.

An element \( v \) of \( \mathcal{H} \) is a square-integrable vector field \( k \mapsto v(k) \) with the value

\[
v(k) = \sum_{n \in \mathbb{N}_0} \sum_{\iota \in \Gamma^n} c_n(v(k)) \hat{e}_i(k), \quad c_n(v(k)) := \langle \hat{e}_i(k), v(k) \rangle_{\mathcal{H}(k)}
\]

defined for \( \mu \)-a.e. \( k \). Indeed, (2.2) implies

\[
\langle \hat{e}_{\iota'}(k), v(k) \rangle_{\mathcal{H}(k)} = \sum_{n \in \mathbb{N}_0} \sum_{\iota \in \Gamma^n} c_n(v(k)) \langle \hat{e}_{\iota'}(k), \hat{e}_i(k) \rangle_{\mathcal{H}(k)}
\]

with \( \iota' \in \Gamma^{n'} \). But, using (2.1)

\[
\langle \hat{e}_{\iota'}(k), \hat{e}_i(k) \rangle_{\mathcal{H}(k)} = \frac{\delta_{n'n'}}{n!'n'} \sum_{\pi \in \mathfrak{S}_n} \delta_{\iota', \pi \iota}
\]

and \( \delta_{\iota', \pi \iota} \) is the product of Kronecker symbols \( \delta_{\lambda_1 \lambda_1', \lambda_2 \rho_1} \cdots \delta_{\lambda_n \lambda_n', \rho_n \rho_n'} \), abbreviated as \( \delta_{n\iota \iota'} \cdots \delta_{n'\iota' \iota'} \). Now use the fact that the coordinate \( c_n(v(k)) \) of \( v(k) \in \mathcal{H}(k) \) is invariant under the action of \( \mathfrak{S}_n \).
Using (3.3) and relation (2.3)

\[ \| b_{i_1}(k) v(k) \|_{\mathcal{H}(k)} \leq C_0 \| v(k) \|_{\mathcal{H}(k)} \]

where the constant \( C_0 \geq 1 \) depends only on a field \( v \).

The formal adjoint of \( b_{i_1}(k) \) coincides with the adjoint \( b_{i_1}(k)^\ast \), which is called the annihilation operator. Using (2.1) and (3.1)

\[ b_{i_1}(k)^\ast v(k) = \sum_{n \in \mathbb{N}} \sqrt{n} \sum_{i \in \mathbb{N}^{n-1}} c_{i_1}(v(k)) e_i(k). \]

Using (2.1) and (3.3), the definition of the coordinate \( c_{i_1}(v(k)) \) in (2.2), and then applying the Cauchy–Schwarz inequality and relation (2.3)

\[ \| b_{i_1}(k)^\ast v(k) \|_{\mathcal{H}(k)} \leq C_0' \| v(k) \|_{\mathcal{H}(k)} \]

where the constant \( C_0' \geq 0 \) depends only on \( v \).

Using (3.1) and (3.3)

\[ \sum_{i_1 \in I} b_{i_1}(k) b_{i_1}(k)^\ast = n(k) \quad \text{where} \quad n(k) v(k) = \sum_{n \in \mathbb{N}_0} n v_n(k) \]

and the sum over \( i_1 \) is understood as a strong limit of partial sums; the creation/annihilation operators satisfy the commutation relations

\[ [b_{i_1}(k)^\#, b_{i_2}(k)^\#] = 0, \quad [b_{i_1}(k)^\ast, b_{i_2}(k)] = \delta_{i_1,i_2} I(k) \]

for \( i_1, i_2 \in I \). Here \( b_{i_1}(k)^\# \) denotes either \( b_{i_1}(k) \) or \( b_{i_1}(k)^\ast \).

By definition, for every \( v \in \mathcal{H} \), the field \( k \mapsto b_{i_1}(k)^\# v(k) \) is measurable. Thus the field \( k \mapsto b_{i_1}(k)^\# \) of bounded operators is measurable, and it defines a bounded decomposable operator \( b_{i_1}^\# = \int \oplus b_{i_1}(k)^\# \mu(dk) \) [17, Definition II.2.3.2], called the creation/annihilation operator in \( \mathcal{H} \). Let \( n(k) \in \mathcal{B}(\mathcal{H}(k)) \) be as in (3.5). A bounded self-adjoint operator \( n = \int \oplus n(k) \mu(dk) \) is called the number operator. Interpreting \( b_{i_1}^\# \) as the creation/annihilation operator of the \( i_1 \)th phonon state, one concludes that the number operator \( n \) is the sum of occupation numbers \( b_{i_1} b_{i_1}^\ast \) of phonon states, i.e. \( n \) is the total-number operator.
Let $k \mapsto \omega(k)$ be a continuous nonnegative function such that the field $k \mapsto \omega(k)I(k)$ is measurable. A diagonalizable operator

$$
\omega = \int \omega(k)I(k)\mu(dk)
$$

defined on the domain

$$
\text{dom } \omega = \{v \in \mathbb{R} | \omega(k)v(k) \in \mathbb{R}(k) \text{ } \mu\text{-a.e., } \int \|\omega(k)v(k)\|^2_{\mathbb{R}(k)}\mu(dk) < \infty\}
$$
is self-adjoint. We call the operator $n\omega$ on dom $\omega$ the kinetic energy of phonons.

For future reference, let us remark the following.

**Proposition 3.1.** When $k \mapsto \omega(k)$ is of class $L^2(\mathbb{R}^+, \mu)$, dom $\omega = \mathbb{R}$.

This is merely due to Hölder inequality [22, Theorem 2.4 and Corollary 2.5].

### 3.2. Kinetic energy of a molecule

Let $\mathcal{L}_0$ be a separable complex Hilbert space with an orthonormal basis $(w_{JM}); M \in I_J := \{-J, \ldots, J\}, J \in \mathbb{N}_0$. $\mathcal{L}_0$ admits a decomposition, $\mathcal{L}_0 = \bigoplus_i \mathcal{L}_{0,i}$, where each Hilbert space $\mathcal{L}_{0,i}$ has the basis $(w_{JM})_M$. The kinetic energy of a molecule is described as follows. Let $J_x$, with $x \in \{1, 2, 3\}$, be the $\mathfrak{su}_2$-algebra representation on $\mathcal{L}_{0,i}$ corresponding to the $x$th generator of $\mathfrak{su}_2$. The action of $J_x$ on $\mathcal{L}_{0,i}$ is defined as in [11, Eq. (14.5)]; so $J_x$ is simple (or else reducible). Considering $\mathcal{L}_{0,i}$ as a vector space, one extends $J_x \in \text{End } \mathcal{L}_{0,i}$ to $\mathcal{L}_0$ by linearity. The extensions form the vector-valued operator $J = (J_1, J_2, J_3)$ referred to as the angular momentum operator of a linear-rotor impurity. The operator $J^2 = JJ$ defined on its maximal domain reads

$$
J^2 = \sum_{J \in \mathbb{N}_0} \sum_{M \in I_J} J(J + 1)w_{JM}^\dagger \otimes w_{JM}, \quad \text{dom } J^2 = \{w \in \mathcal{L}_0 | J^2w \in \mathcal{L}_0\}
$$

where $(w_{JM}^\dagger)$ is the adjoint basis. One identifies $w_{JM}^\dagger \otimes w_{JM} : \mathcal{L}_0 \to \mathcal{L}_0$ with a rank one projection $\langle w_{JM}^\dagger, w_{JM} \rangle_{\mathcal{L}_0} w_{JM}$. The operator $J^2$ is written in its spectral representation, hence it is self-adjoint. For $c > 0$, $cJ^2$ is called the kinetic energy of a molecule.

### 3.3. Phonon excitations

Let $\mathcal{H} := \mathcal{L}_0 \otimes \mathbb{R}$ be the Hilbert tensor product. Consider the constant field $k \mapsto \mathcal{L}(k)$ of complex Hilbert spaces corresponding to $\mathcal{L}_0$. That is, $\mathcal{L} = \int \mathcal{L}(k)\mu(dk)$ coincides with $L^2(\mathbb{R}^+, \mu; \mathcal{L}_0)$. Then $\int \mathcal{L}(k)\mu(dk)$, with $\mathcal{H}(k) := \mathcal{L}(k) \otimes \mathbb{R}(k)$, is isomorphic to $\mathcal{H}$ [17, Sec. 2.1.8] and therefore will be identified with $\mathcal{H}$ in what follows.

Let $\lambda \in \mathbb{N}_0$ and let $U^\lambda: k \mapsto U^\lambda(k)$ be a nonnegative measurable function. Let us define

$$
\begin{align*}
U & : k \mapsto U^\lambda(k) := \sum_{\lambda \in \mathbb{N}_0} (2\lambda + 1)^{3/2}U^\lambda(k), \\
\mathfrak{U} & := \{v \in \mathbb{R} | U^\lambda(k)v(k) \in \mathbb{R}(k) \mu\text{-a.e.}, \int \|U^\lambda(k)v(k)\|^2_{\mathbb{R}(k)}\mu(dk) < \infty\}.
\end{align*}
$$

**Remark 3.2.** Similar to Proposition 3.1, if $U \in L^2(\mathbb{R}^+, \mu)$ then $\mathfrak{U} = \mathbb{R}$.

Let $I_0$ be the identity map in $\mathcal{L}_0$ and consider the operator in $\mathcal{H}$ defined by

$$
Q := \sum_{\lambda \in \mathbb{N}_0} \sum_{\rho \notin I_\lambda} Y_{\lambda, -\rho}(\partial)I_0 \otimes U^\lambda_{\lambda, \rho}, \quad \text{dom } Q = \{\psi \in \mathcal{H} | Q\psi \in \mathcal{H}\}.$$

\[ (3.9b) \quad U_{\lambda p} := \int_\mathbb{R}^2 U_{\lambda p}(k) \mu(dk), \quad U_{\lambda p}(k) := U_\lambda(k)b_{\lambda p}(k). \]

The infinite sum over \( \lambda \) is understood as a strong limit of partial sums. The spherical harmonic \( Y_{\lambda p}(\hat{\alpha}) \) depends on the molecular orientation given in terms of the spherical angles \( \hat{\alpha} \); i.e., the commutator \([J_x, Y_{\lambda p}(\hat{\alpha})]\) is calculated using \([11, \text{Eq. (14.13)}], \ [12, \text{Eq. (3.53)}] \).

**Lemma 3.3.** \( \mathcal{L}_0 \otimes \mathcal{U} \subseteq \text{dom } Q. \)

**Proof.** Let \( w \otimes v \in \mathcal{S} \). By \((3.9)\), and then using the Cauchy–Schwarz inequality
\[
\|Q(w \otimes v)\|_{\mathcal{S}}^2 \leq \int_\mathbb{R}^2 \sum_{\lambda, \rho} \|Y_{\lambda, -\rho} w\|_{\mathcal{L}_0} \|U_{\lambda p}(k)v(k)\|_{H(k)}^2 \mu(dk).
\]
Using \( \|Y_{\lambda p} w\|_{\mathcal{L}_0} \leq (2\lambda + 1)/(4\pi)\|w\|_{\mathcal{L}_0} \), it follows from \((3.2)\) and \((3.8)\) that
\[
\|Q(w \otimes v)\|_{\mathcal{S}} \leq (4\pi)^{-1/2} C_v \|w\|_{\mathcal{L}_0} \left( \int \|U(k)v(k)\|_{H(k)}^2 \mu(dk) \right)^{1/2}.
\]
Therefore \( w \otimes v \in \mathcal{L}_0 \otimes \mathcal{U} \Rightarrow w \otimes v \in \text{dom } Q. \)

**Hypothesis 3.4.** \( k \mapsto \omega(k) \) and \( k \mapsto U(k) \) are of class \( L^\infty(\mathbb{R}^+, \mu). \)

Yet Hypothesis 3.4 encloses the physically interesting cases. We thus have that \( Q \in \mathcal{B}(\mathcal{S}) \) is a bounded operator in \( \mathcal{S} \). Then, the operator
\[
(3.10) \quad W := Q + Q^* \quad \text{is bounded, self-adjoint, and decomposable relative to the field } k \mapsto \mathcal{S}(k). \quad \text{The operator } W \text{ describes phonon excitations and is referred to as the impurity-boson interaction potential (cf. (1.1)).}
\]

### 3.4. Angulon operator.

Using Hypothesis 3.4, the operator
\[
(3.11) \quad A^0 := cJ^2 \otimes I + I_0 \otimes n\omega
\]
is a self-adjoint operator defined on \( \text{dom } A^0 = \text{dom } J^2 \otimes \mathcal{R} \). The operator
\[
(3.12) \quad A := A^0 + W, \quad \text{dom } A = \text{dom } A^0
\]
is called the **angulon operator**. Since \( W = \int_\mathbb{R}^2 W(k) \mu(dk) \) is bounded decomposable and \( A^0 = \int_\mathbb{R}^2 A^0(k) \mu(dk) \) is self-adjoint decomposable, the angulon operator \( A = \int_\mathbb{R}^2 A(k) \mu(dk) \) is decomposable \([23]\) with \( A(k) := A^0(k) + W(k) \). Since \( \text{dom } (A^0 + W) = \text{dom } A^0 \), the operator sum \( A \) of two self-adjoint operators \( A^0 \) and \( W \) is self-adjoint.

### 4. Rotated angulon operator.

By definition \((3.12)\), the angulon operator \( A = A(\hat{\alpha}) \) depends on the molecular orientation, as defined by the spherical angles \( \hat{\alpha} = (\vartheta, \varphi) \). Here we show that, with a suitable choice of \( \hat{\alpha}' \), the operator \( A' = A(\hat{\alpha}') \) is unitarily equivalent to \( A \) and it commutes with rotations in \( \mathcal{S} \). It is this result that eventually implies that the angulon is an eigenstate of the total angular momentum \( L \) of the system.

By construction, the vector space \( V(k) \) admits a decomposition \( \otimes \lambda V_\lambda(k) \). Similar to \( J_x \) on \( \mathcal{L}_0 J \), we let \( \Lambda_x \), with \( x \in \{1, 2, 3\} \), be a simple \( \mathfrak{su}_2 \)-algebra representation on \( V_\lambda(k) \). We denote by \( M(R) \) be the rotation operator generated by \( \{\Lambda_1, \Lambda_3\} \) \([12, \text{Eq. (3.53)}]\).
Eq. (3.8). Here $R = R(\Phi, \Theta, \Psi)$ is a rotation matrix of $SO_3$ parametrized by Euler angles.

Using (3.1), $e_\epsilon(k) = b_\epsilon(k)1(k)$ for $\epsilon \in I$. Therefore $b_{\lambda, \rho}(k)$ is the $\rho$th component of a rank-$\lambda$ irreducible tensor operator $b_\lambda(k)$ in the sense of Fano–Racah [11, 12]. Unlike $b_\lambda(k)$, the adjoint operator $b_{\lambda, \rho}(k)^*$ does not transform as the irreducible tensor operator, since there arises an additional phase factor in the complex conjugate of the Wigner $D$-function $D_{\mu \rho}(R)$, i.e. $D_{\mu \rho}(R) = (-1)^{\mu-\rho'} D_{-\rho, -\rho}(R)$ for $\rho, \rho' \in \Gamma_\lambda$ (see e.g. [11, Eqs. (2.19) and (2.21)]). However, the operator

\begin{equation}
(4.1) b_{\lambda, \rho}(k)^* := (-1)^{\lambda-\rho} b_{\lambda, -\rho}(k)^*
\end{equation}

does define the $\rho$th component of a rank-$\lambda$ irreducible tensor operator $b_\lambda(k)^*$. Here the extra phase $(-1)^{\lambda}$ is introduced for convenience.

The tensor product module $\mathbb{L}_{0, j} \otimes V_\lambda(k)$ is the tensor product vector space with the action of $\mathfrak{su}_2$ determined by the relation

\begin{equation}
(4.2) L_x(w \otimes v(k)) = J_x w \otimes v(k) + w \otimes J_x v(k)
\end{equation}

for $w \otimes v(k) \in \mathbb{L}_{0, j} \otimes V_\lambda(k)$. Similar to $M(R)$, let $L(R)$ and $K(R)$ be the rotation operators generated by \{J_1, J_3\} and \{L_1, L_3\}, respectively. Using (4.2)

\begin{equation}
(4.3) K(R) = L(R) \otimes M(R).
\end{equation}

By linearity, a unitary $K(R)$ extends to the operator in $\mathbb{L}_0 \otimes V(k)$.

Given two simple modules, $V_\lambda(k)$ and $V_{\lambda'}(k)$, the tensor product module $V_\lambda(k) \otimes V_{\lambda'}(k)$ is the tensor product vector space with the action of $\mathfrak{su}_2$ determined by the condition

$$
\Lambda_x (v(k) \otimes u(k)) = \Lambda_x v(k) \otimes u(k) + v(k) \otimes \Lambda_x u(k)
$$

for $v(k) \otimes u(k) \in V_\lambda(k) \otimes V_{\lambda'}(k)$. The tensor product of finitely many $\mathfrak{su}_2$-modules is defined analogously. Using the latter, $K(R)$ extends to the unitary operator in $\mathbb{L}_0 \otimes \mathbb{R}(k)$. There exists a unique isomorphism mapping $w \otimes v \in \mathbb{L}_0 \otimes \mathbb{R}$ into the field $k \mapsto w \otimes v(k)$; so the operator

$$
K(R) := \int_0^\pi K(R_\delta) \mu(d\delta)
$$

is a unitary decomposable operator in $\mathbb{L}$.

Let $R_\delta := R(\varphi + \pi/2, \vartheta, 0)$. According to [11], this particular $R_\delta$ is useful in that it gives

\begin{equation}
(4.4) Y_{\lambda, \rho}(\delta) = \sqrt{(2\lambda + 1)/(4\pi)} D_{\rho \rho}(R_\delta) \quad \text{and} \quad \overline{Y_{\lambda, \rho}(\delta)} = Y_{\lambda, -\rho}(\delta')
\end{equation}

for $\delta' = \delta \pm (0, \pi)$ mod $(0, 2\pi)$. Let us define

\begin{equation}
(4.5) A' = A'(\delta) := K(R_\delta) A(\delta) K(R_\delta)^*
\end{equation}

and call $A'$ the rotated angulon operator. We have that

**Theorem 4.1.** $A'(\delta) = A'(\delta')$.

An immediate consequence of Theorem 4.1 is that $A'$ is the $SO_3$-scalar tensor operator. To see this, put $Y_{\lambda, \rho}(\delta') = (-1)^{\rho} Y_{\lambda, \rho}(\delta)$ in $A'(\delta')$ and sum over $\rho \in \Gamma_\lambda$. Applying the rules for reducing the tensor product $[\lambda] \otimes [\lambda]$ of $SO_3$-irreducible representations

$$
\sum_{\rho \in \Gamma_\lambda} Y_{\lambda, -\rho}(\delta') I_0 \otimes b_{\lambda, \rho}(k) = (-1)^{\lambda} \sqrt{2\lambda + 1} \{ Y_{\lambda}(\delta) I_0 \otimes b_\lambda(k) \}_0
$$

The result is $A'(\delta') = A'(\delta)$.
where \( \{Y_\lambda(\hat{o})I_0 \otimes b_\lambda(k)\}_0 \) is a rank-0 \( SO_3 \)-irreducible tensor operator. With the help of (4.1), the same is done for the adjoint operator. By (3.9)–(3.12)

\[
A' = A' + W', \quad W' = \int \otimes W'(k) \mu(\text{dk}) \quad \text{with}
\]

\[
W'(k) := \sum_{\lambda \in \mathbb{N}_0} \sqrt{2\lambda + 1} U_\lambda(k)((-1)^\lambda \{Y_\lambda \otimes b_\lambda(k)\}_0 + \{Y_\lambda \otimes b_\lambda(k)^{\sim}\}_0)
\]

where \( Y_\lambda = Y_\lambda(\hat{o}) \) and, for simplicity, we omit \( I_0 \).

**Proof of Theorem 4.1.** Since \( A' \) is invariant under rotations in \( \hat{\mathfrak{g}} \), it suffices to examine \( W \). Using the tensor structure of measurable fields \( k \mapsto b_\lambda(k) \) and \( k \mapsto b_\lambda(k)^{\sim} \), one writes \( W(k) \) as a sum of rank-L tensor operators

\[
W(k) = \sum_{\lambda \leq L} U_\lambda(k)x_{\lambda L}(\{Y_\lambda(\hat{o}) \otimes b_\lambda(k)\}_{L0} + (-1)^\lambda \{Y_\lambda(\hat{o}) \otimes b_\lambda(k)^{\sim}\}_{L0})
\]

where \( L \in \{0, 2, \ldots, 2\lambda\} \) and \( x_{\lambda L} \) is the sum of Clebsch–Gordan coefficients:

\[
x_{\lambda L} := \sum_\rho \begin{bmatrix} \lambda & \lambda & L \\ -\rho & \rho & 0 \end{bmatrix}.
\]

Let \( b_{\lambda\rho}(k)^\# \) denote either \( b_{\lambda\rho}(k) \) or \( b_{\lambda\rho}(k)^{\sim} \). Using (4.3)

\[
K(R)^*(Y_{\lambda,-\rho}(\hat{o})I_0 \otimes b_{\lambda\rho}(k)^\#)K(R)
\]

\[
= \sum_{\rho'} D_{\rho',\rho}(R)Y_{\lambda\rho'}(\hat{o})I_0 \otimes \sum_{\rho''} D_{\rho''\rho}(R)b_{\lambda\rho''}(k)^\#.
\]

Now choose \( R = R_{\hat{o}}^{-1} \). Using (4.4), the sum over \( \rho' \in I_\lambda \) gives a factor \( \delta_{\rho 0} \) and

\[
K(R_{\hat{o}})\{Y_\lambda(\hat{o})I_0 \otimes b_\lambda(k)^\#\}_{L0}K(R_{\hat{o}})^*
\]

\[
= \begin{bmatrix} \lambda & \lambda & L \\ 0 & 0 & 0 \end{bmatrix} \sum_{L'} x_{\lambda L'}\{Y_\lambda(\hat{o}')I_0 \otimes b_\lambda(k)^\#\}_{L'0}.
\]

Apply (4.8) to (4.7) and calculate the sum over \( L \), which is 1. Using (4.5), conclude that \( A'(\hat{o}) = A(\hat{o}) \).

Since the operators \( A' \) and \( A \) are unitarily equivalent, hereafter we identify \( A' \) (resp. \( W' \)) with \( A \) (resp. \( W \)).

5. **Field of orthonormal bases**

Here we construct the field of orthonormal bases of \( \mathfrak{g}(k) \) that transform under rotations as an irreducible tensor operator.

By construction, \( T(V(k)) = \oplus_\lambda T(V_\lambda(k)) \) as a vector space. The ideal \( I(V(k)) \) is homogeneous in the sense that it obeys the form \( \oplus_\lambda I(V_\lambda(k)) \), where \( I(V_\lambda(k)) \) denotes \( I(V(k)) \cap T(V_\lambda(k)) \). Thus

\[
S(V(k)) = \oplus_\lambda S(V_\lambda(k)), \quad S(V_\lambda(k)) := T(V_\lambda(k))/I(V_\lambda(k)).
\]

We explore this fact below.

For \( \iota = ((\lambda, \rho_1), \ldots, (\lambda, \rho_n)) \), \( \rho = (\rho_1, \ldots, \rho_n) \in I_\lambda^n \), put

\[
\hat{e}_{\lambda \rho}(k) := \hat{e}_i(k).
\]

When \( n = 0 \), \( \rho = \rho_0 \) is empty and \( \hat{e}_{\lambda \rho}(k) := 1(k) \). Thus

\[
(\hat{e}_{\lambda \rho}(k) | \rho \in I_\lambda^n)_{n \in \mathbb{N}_0}
\]
is the basis of $S(V_\lambda(k))$.

Further, for $\ell' = ((\lambda, \rho_1'), \ldots, (\lambda, \rho_{\ell'})$, $\rho' = (\rho_1', \ldots, \rho_{\ell'}) \in \Gamma_\lambda'$, put

$$\hat{e}_{\lambda_{\ell'}^{\rho'}}(k) := \hat{e}_{\ell'}(k).$$

The action of $\mathfrak{S}_n$ on $\rho \in \Gamma_\lambda$ is defined similar to that of $\mathfrak{S}_n$ on $\ell \in \Gamma^n$.

5.1. SCFP. Let $\Gamma_\lambda$ be the set of pairs

$$\gamma := (\Lambda, M), \quad M \in \Gamma_\lambda := \{-\Lambda, -\Lambda + 1, \ldots, \Lambda\}$$

where $\Lambda$ is obtained by reducing the tensor product of $n$ copies of $SO_3$-irreducible representations $[\lambda]$. We look for a transformation—as a collection of coefficients $c_\rho(\Lambda^n\gamma) \in \mathbb{C}$—that maps a measurable field $k \mapsto v_{\lambda^n\gamma}(k)$ of orthonormal bases onto the field of bases in (5.2):

$$\hat{e}_{\lambda^n\gamma}(k) = \sum_{\gamma \in \Gamma_\lambda} c_\rho(\Lambda^n\gamma)v_{\lambda^n\gamma}(k).$$

By (5.3), $c_\rho(\Lambda^n\gamma)$ is invariant under the action of $\mathfrak{S}_n$. When $n = 0$ and $n = 1$, (5.3) is trivial

\begin{align*}
(5.4a) \quad c_{\rho_1}(\Lambda^0\Lambda M) := & \delta_{\Lambda^0\delta_{M^0}}, \quad v_{\lambda^n\Lambda M}(k) := \delta_{\Lambda^0\delta_{M^0}} 1(k), \\
(5.4b) \quad c_{\rho_1}(\Lambda^1\Lambda M) := & \delta_{\Lambda^2\delta_{M^2}}, \quad v_{\lambda^n\Lambda M}(k) := \delta_{\Lambda^2\delta_{M^2}} v_{\lambda^n\gamma}(k).
\end{align*}

We require $(v_{\lambda^n\gamma}(k))$ to be an orthonormal basis of $\mathfrak{H}(k)$. By (5.4a), $v_{\lambda^n\gamma}(k)$ is an element of $T^0(V(k))$ and it does not depend on $\lambda$. Thus we have

\begin{align*}
(5.5a) \quad \langle v_{\lambda^n\gamma}(k), v_{\lambda^n\gamma'}(k) \rangle_{\mathfrak{H}(k)} = & \delta_{nn'}\delta_{\gamma\gamma'}\delta_{\Lambda\Lambda'}, \quad n, n' \in \mathbb{N}, \\
(5.5b) \quad \langle v_{\lambda^n\gamma}(k), 1(k) \rangle_{\mathfrak{H}(k)} = & \delta_{nn'\gamma}e_{\Lambda}\delta_{M0}, \quad n \in \mathbb{N}_0.
\end{align*}

Here and elsewhere, $\delta_{\gamma\gamma'}$ reads $\delta_{\Lambda\Lambda'}\delta_{M'\Lambda}$, and $\delta_{\gamma\gamma}$ reads $\delta_{\Lambda\Lambda\delta_{M^0}}$.

Now assume that $n = 2; \rho = (\rho_1, \rho_2) \in \Gamma_\lambda^*$. We have that $[\lambda] \otimes [\lambda]$ reduces to $[\Lambda]$ for $\Lambda \in \{0, 1, \ldots, 2\lambda\}$. However, using the first commutation relation in (3.6), the basis vector $\{e_{\lambda}(k)\}_{AM}$ of the space of the representation labeled by $[\Lambda]$ vanishes identically for $\Lambda$ odd. That is

$$\{e_{\lambda}(k) \otimes e_{\lambda}(k)\}_{AM} = (-1)^{\lambda + \lambda - \lambda} \{e_{\lambda}(k) \otimes e_{\lambda}(k)\}_{AM}.$$ 

Thus, for $\lambda = \lambda', \Lambda \in \{0, 2, \ldots, 2\lambda\}$. Using the latter, (5.3) holds for

\begin{align*}
(5.6a) \quad c_{\rho_1, \rho_2}(\Lambda^2\Lambda M) := & \langle \lambda\lambda \lambda M \rangle \left[ \begin{array}{ccc} \lambda & \lambda & \Lambda \\
\rho_1 & \rho_2 & M \end{array} \right], \\
(5.6b) \quad v_{\lambda^2\Lambda M}(k) := & \langle \lambda\lambda \lambda \Lambda M \rangle \{e_{\lambda\lambda}(k)\}_{AM}, \quad \langle \lambda\lambda \lambda \Lambda M \rangle := \frac{1 + (-1)^{\Lambda}}{2}.
\end{align*}

A one-to-one correspondence between $(v_{\lambda^n\gamma}(k) | \gamma \in \Gamma^n)$ and (5.2) requires the transformation in (5.3) to have an inverse. We look for the inverse transformation by generalizing (5.6b) by induction

$$v_{\lambda^n\Lambda M}(k) = \sum_{\Lambda'} \{v_{\lambda^{n-1}\Lambda'}(k) \otimes e_{\lambda}(k)\}_{AM}(\lambda^{n-1}\Lambda'\Lambda|\lambda^n\Lambda)$$

and $\Lambda'$ is obtained by reducing the tensor product of $n - 1$ copies of $SO_3$-irreducible representations $[\lambda]$. One assumes that the coefficient satisfies

\begin{align*}
(5.8a) \quad \langle \lambda^0(\Lambda')\lambda|\lambda^1\Lambda \rangle := & \delta_{\Lambda^n\delta_{\Lambda\Lambda}}, \\
(5.8b) \quad \langle \lambda^1(\Lambda')\lambda|\lambda^2\Lambda \rangle := & \delta_{\Lambda^n\Lambda|\lambda^3\Lambda},
\end{align*}
(5.8c) \[(\lambda^{n-1}(\Lambda')\lambda|\lambda^n\Lambda) \equiv (\lambda^n\Lambda|\lambda^{n-1}(\Lambda')\lambda), \quad n \in \mathbb{N}.\]

Then, relation (5.7) holds for all \(n \in \mathbb{N}\), and it is compatible with (5.4) and (5.6b).

The coefficient formally plays the same role as the coefficient of fractional parentage (CFP) in an antisymmetric case of fermionic particles (when describing electron-shells of an atom). Thus we call \((\lambda^{n-1}(\Lambda')\lambda|\lambda^n\Lambda)\) the symmetric coefficient of fractional parentage (SCFP).

### 5.2. Coefficient identities

The properties of the SCFPs are somewhat similar to those of regular CFPs. For our purposes we need only two of them. By (5.5), (5.7)

\[
1 = \sum_{\Lambda'} |(\lambda^{n-1}(\Lambda')\lambda|\lambda^n\Lambda)|^2, \quad n \in \mathbb{N}
\]

(cf. [11, Eq. (9.13)], [27, Eq. (11.9)]). Applying relation (5.7) twice

\[
0 = \sum_{\Lambda_1} \sqrt{2\Lambda_1 + 1} \left\{ \frac{\lambda}{\Lambda_2} \frac{\lambda'}{\Lambda} \right\}
\]

(5.10)

\[
\cdot (\lambda^{n-2}(\Lambda_2)\lambda|\lambda^{n-1}\Lambda_1)(\lambda^{n-1}(\Lambda_1)\lambda|\lambda^n\Lambda), \quad n \in \mathbb{N}_{\geq 2}
\]

for \(\Lambda'\) odd (cf. [11, Eq. (9.12)], [27, Eq. (11.8)]). The coefficient \(\{\cdots\}\) is the 6j-symbol. Using (5.9) and (5.10), and assuming that the SCFPs are real numbers, some numerical values are shown in Tab. 1. There, the SCFPs with missing numbers \(\Lambda, \Lambda'\) allowed by the rules of angular reduction vanish identically.

**Table 1.** Numerical values of some \((\lambda^{n-1}(\Lambda')\lambda|\lambda^n\Lambda)\).

| \(\lambda^{n-1}(\Lambda')\lambda|\lambda^n\Lambda\) | \(\lambda^{n-1}(\Lambda')\lambda|\lambda^n\Lambda\) | \(\lambda^{n-1}(\Lambda')\lambda|\lambda^n\Lambda\) |
|-----------------|-----------------|-----------------|
| \(2^2(0)\)      | \(1\)           | \(\sqrt{5/3}\)  |
| \(2^2(2)\)      | \(1\)           | \(\sqrt{2/1}\)  |
| \(3\)           |                 | \(\sqrt{5/7}\)  |
| \(2^2(0)\)      | \(2\)           | \(\sqrt{7/15}\) |
| \(2^2(2)\)      | \(2\)           | \(\sqrt{2/1}\)  |
|                 |                 | \(4\)           |

By analogy to the recurrence relation (5.10) for the SCFPs, one finds the recurrence relation for the coefficients in (5.3).

**Lemma 5.1.** Let \(\rho_1 \in I_\lambda\) and \(\rho \in I^n\) and \((\Lambda, M) \in \Gamma_{\lambda^{n+1}}\) and \(n \in \mathbb{N}_0\). Then

\[
c_{\rho\rho_1}(\lambda^{n+1}\Lambda M) = \sum_{(\Lambda', M') \in \Gamma_{\lambda^{n}}} c_{\rho}(\lambda^{n}\Lambda' M')(\lambda^{n+1}\Lambda|\lambda^n(\Lambda')\lambda) \left[ \Lambda' \lambda \rho_1 \Lambda \right].
\]

**Proof.** By (5.4) and (5.6a), it suffices to examine the case \(n \geq 2\). Using (3.1) and then (5.3)

\[
(5.11) \quad b_{\lambda\rho_1}(k)\hat{e}_{\lambda^n\rho}(k) = \sqrt{n + 1} \sum_{\gamma \in \Gamma_{\lambda^{n+1}}} c_{\rho\rho_1}(\lambda^{n+1}\gamma) v_{\lambda^{n+1}\gamma}(k).
\]

On the other hand, using (5.3) and then (3.1)

\[
(5.12) \quad b_{\lambda\rho_1}(k)\hat{e}_{\lambda^n\rho}(k) = \sqrt{n + 1} \sum_{\gamma \in \Gamma_{\lambda^n}} c_{\rho}(\lambda^{n}\gamma) v_{\lambda^n\gamma}(k) \otimes e_{\lambda\rho_1}(k).
\]
We argue by induction. Assume that the sum over
\( (5.16) \)
Proof. We show that the field of orthonormal bases
\( \) 
\( \) 
\( \) 
\( (5.17b) \)
Next, using \((5.5a)\) and \((5.7)\)
The latter together with \((5.9)\) implies
\( (5.14) \)
Substitute \((5.14)\) in \((5.13)\) and deduce the relation as claimed.
\[ \sum_{c \in I^\lambda} c_r(\lambda^n\gamma) = \delta_{\gamma',\gamma}. \]
\[ (5.15) \]
Proof. Let \( \rho_1 \in I^{\lambda}_n \) and \( \rho \in I^\lambda_{n+1} \) and \( \gamma_1, \gamma_2 \in \Gamma^\lambda_{n+1} \). By Lemma 5.1
\begin{align*}
\sum_{\rho, \rho_1} c_{\rho, \rho_1}(\lambda^{n+1}\gamma_1) & = \sum_{\gamma_1, \gamma_2 \in \Gamma^\lambda_{n+1}} (\lambda^n A_2 \| \lambda^n A_1 \| \lambda^n A_1) \\
& \cdot \sum_{\rho_1} \left[ \frac{A_1}{M_1} \frac{A_2}{M_2} \right] \sum_{\rho} c_{\rho}(\lambda^{n+1}\gamma_2) c_{\rho}(\lambda^n\gamma_1).
\end{align*}
\[ (5.16) \]
We argue by induction. Assume that the sum over \( \rho \) on the right-hand side is \( \delta_{\gamma',\gamma} \). Then, using \((5.9)\), the right-hand side of \((5.16)\) is \( \delta_{\gamma_1,\gamma_2} \). That is, if \((5.15)\) holds for \( c_r(\lambda^n\gamma) \) with \( \rho \in I^\lambda\gamma \), \( \gamma \in \Gamma^\lambda_n \), then \((5.15)\) holds for \( c_r(\lambda^{n+1}\gamma) \) with \( \rho \in I^{\lambda+1}_n \), \( \gamma \in \Gamma^{\lambda+1}_n \). Now, we know from \((5.6a)\) that \((5.15)\) is valid for \( n = 2 \). Thus, \((5.15)\) holds for all \( n \geq 2 \). For \( n = 0 \) and \( n = 1 \), \((5.15)\) applies trivially; see \((5.4)\).

5.3. Hilbert space decomposition. With the help of the previously obtained results one deduces the following.

**Theorem 5.3.** The sequence
\[ (1, (v_{\lambda^*\gamma} \mid \gamma \in \Gamma^\lambda_n)_{(\lambda,n) \in \mathbb{N}_0 \times \mathbb{N}}) \] 
with
\[ v_{\lambda^*\gamma} = \sum_{\rho \in I^\lambda} c_{\rho}(\lambda^n\gamma) \dot{e}_{\lambda^*\rho} \]
is a measurable field of orthonormal bases of \( \tilde{R}(k) \).

Proof. We show that the field of orthonormal bases
\[ (5.17a) \]
\[ (5.17b) \]
is in one-to-one correspondence with a measurable field of bases in \((5.2)\). Then the proof is accomplished by using \((5.1)\), since \((B_\lambda(k))_{\lambda \in \mathbb{N}_0}\) is a sequence of orthonormal vectors by \((5.5)\).
Relation (5.17b) follows from (5.3) and Corollary 5.2. We show the converse. Multiply (5.17b) by $c_\rho(\lambda^n \gamma)$ and sum over $\gamma \in \Gamma_{\lambda^n}$. We have

$$
\sum_\gamma c_\rho(\lambda^n \gamma) v_{\lambda^n \gamma}(k) = \sum_{\rho'} C_{\lambda^n \rho \rho'} \hat{e}_{\lambda^n \rho}(k)
$$

with

$$
C_{\lambda^n \rho \rho'} := \sum_\gamma c_\rho(\lambda^n \gamma)c_{\rho'}(\lambda^n \gamma).
$$

On the other hand, projecting (5.17b) on $\hat{e}_{\lambda^n \rho}(k)$ and then using (2.1) and that $c_\rho(\lambda^n \gamma)$ is invariant under the action of $\mathfrak{S}_n$

$$
c_\rho(\lambda^n \gamma) = \langle v_{\lambda^n \gamma}(k), \hat{e}_{\lambda^n \rho}(k) \rangle_{\mathfrak{R}(k)}.
$$

By assumption, $B_\lambda(k)$ is complete; hence

$$
C_{\lambda^n \rho \rho'} = \sum_\gamma \langle \hat{e}_{\lambda^n \rho'}(k), v_{\lambda^n \gamma}(k) \rangle_{\mathfrak{R}(k)} \langle v_{\lambda^n \gamma}(k), \hat{e}_{\lambda^n \rho}(k) \rangle_{\mathfrak{R}(k)} = \frac{1}{n!} \sum_{\pi \in \mathfrak{S}_n} \delta_{\rho', \pi \rho}.
$$

Thus, (5.17a) is in one-to-one correspondence with (5.2).

The key conclusion following from Theorem 5.3 is that $\mathfrak{R}$ is the orthogonal sum $\bigoplus \mathfrak{R}_J$ of irreducible invariant subspaces $\mathfrak{R}_J$ spanned by square-integrable vector fields

$$
\{1, v_M | M \in I_\Lambda\}, \quad I = (\lambda^n, \Lambda), \quad n \in \mathbb{N}.
$$

Further, using the rules for reducing the tensor product $[J] \otimes [\Lambda] \to [L]$, the space $\mathfrak{S}_{0,J} \otimes \mathfrak{R}_L$ is the orthogonal sum $\bigoplus_L \mathfrak{S}_{J,LM}$ of irreducible invariant subspaces spanned by square-integrable vector fields

$$
\{w_{LM} | M \in I_L\}, \quad h_{J,LM} := \{w_J \otimes v_T | LM\}.
$$

Therefore

$$
\mathfrak{S}_J = \mathfrak{S}_0^0 \oplus \mathfrak{S}_c^c
$$

where

$$
\mathfrak{S}_0^0 := \bigoplus_L \mathfrak{S}_L^0, \quad \mathfrak{S}_L^0 := \mathfrak{S}_{0,L} \otimes \mathfrak{C}1,
$$

$$
\mathfrak{S}_c^c := \bigoplus_L \mathfrak{S}_L^c, \quad \mathfrak{S}_L^c := \bigoplus_{J,LM} \mathfrak{S}_{J,LM}.
$$

Physically, $\mathfrak{S}_0^0$ is the Hilbert space of vector fields without phonons ($n = 0$); $\mathfrak{S}_c^c$ is the Hilbert space of vector fields that account for phonon excitations ($n \geq 1$).

The spaces $\mathfrak{S}_L^0$ and $\mathfrak{S}_L^c$ are direct integrals of measurable fields $k \mapsto \mathfrak{S}_{0,L} \otimes \mathfrak{C}1(k)$ and $k \mapsto \mathfrak{S}_{L}^c(k)$, respectively, of Hilbert spaces over $(\mathbb{R}^+, \mathfrak{F}, \mu)$. The space $\mathfrak{S}_J^0(k)$ has an orthonormal basis $(w_{LM} \otimes 1(k))_{LM}$; $\mathfrak{S}_J^c(k)$ is the orthogonal sum of Hilbert spaces $\mathfrak{S}_{J,LM}(k)$ with orthonormal bases $(h_{J,LM}(k))_{LM}$. 
We have that
\[(5.19d) \quad \mathcal{H} = \bigoplus_{L} \mathcal{H}_{L}, \quad \mathcal{H}_{L} := \mathcal{H}_{L}^{0} \oplus \mathcal{H}_{L}^{\pm}.
\]
Using (5.19), an element \(\psi_{LM} \) of \(\mathcal{H}_{L} \) is a vector field \(k \mapsto \psi_{LM}(k) \), with the value
\[(5.20a) \quad \psi_{LM}(k) = c_{LM}(k)w_{LM} \otimes 1(k) + \sum_{J,L} c_{JLML}(k) h_{JLML}(k)
\]
belonging to \(\mathcal{H}_{L}(k)\) for \(\mu\)-a.e. \(k\). The sum over \((J,L) \in \mathbb{Z}\) (an index set) is a vector norm limit of partial sums. The coordinates
\[(5.20b) \quad c_{LM}(k) \equiv c_{L=0\Omega_{LM}}(k) := \langle w_{LM} \otimes 1(k), \psi_{LM}(k) \rangle_{\mathcal{H}(k)},
\]
\[(5.20c) \quad c_{JLML}(k) := \langle h_{JLML}(k), \psi_{LM}(k) \rangle_{\mathcal{H}(k)}, \quad n \in \mathbb{N}
\]
are such that
\[(5.20d) \quad k \mapsto (c_{LM}(k))_{M \in \mathbb{N}} \text{ is of class } L^{2}(\mathbb{R}^{+}, \mu; \ell^{2}(I_{L})),
\]
\[(5.20e) \quad k \mapsto (c_{JLML}(k))_{(J,L) \in \mathbb{Z} \times 1_{L}} \text{ is of class } L^{2}(\mathbb{R}^{+}, \mu; \ell^{2}(Z \times 1_{L})).
\]
According to (2.3), there exists a finite \(N \in \mathbb{N}_{0}\) such that \(c_{JLML}(k)\) vanishes identically for \(n > N\). Thus, the sum over \(n \in \mathbb{N}\) in (5.20a) is actually the sum over \(n \in \{1, 2, \ldots, N\}\) for some finite \(N\).

An element \(\psi\) of \(\mathcal{H}\) is a vector field \(k \mapsto \psi(k)\), with the value given by the linear span of (5.20a).

6. DECOMPOSITION OF ANGULON OPERATOR

Here we calculate the matrix elements of the (rotated) angulon operator (4.6) with respect to the field (5.18) of orthonormal bases of \(\mathcal{H}_{L}(k) \oplus \mathcal{H}_{JL}(k)\); here and elsewhere, we assume that \(n \in \mathbb{N}\) when we write \(\mathcal{H}_{JL}(k)\). The results have direct influence on the spectral analysis of angulon.

The orthonormal bases represent the \(SO_{3}\)-irreducible tensor operator of rank \(L\).

Since the angulon operator \(A\) is the \(SO_{3}\)-scalar tensor operator, the Wigner–Eckart theorem [11, Eq. (5.15)], [12, Eq. (3.41)], [27, Sec. I.2] implies that the matrix elements of \(A\) are diagonal with respect to \((L, M_{L})\). Thus \(A\) maps \(\text{dom } A \cap \mathcal{H}_{L}\) into \(\mathcal{H}_{L}\), i.e. \(\mathcal{H}_{L}\) is an invariant subspace for \(A\). Then, the operator
\[(6.1) \quad A_{L} := A|_{\text{dom } A_{L}}, \quad \text{dom } A_{L} := \text{dom } A \cap \mathcal{H}_{L}
\]
is the part of \(A\) in \(\mathcal{H}_{L}\). The domain \(\text{dom } A_{L}\) consists of measurable vector fields \(k \mapsto \psi_{LM}(k)\), with \(\psi_{LM}(k)\) as in (5.20), and with the coordinates satisfying in addition the property that
\[(6.2a) \quad k \mapsto (L(L+1)c_{LM}(k))_{M \in \mathbb{N}} \text{ is of class } L^{2}(\mathbb{R}^{+}, \mu; \ell^{2}(I_{L})),
\]
\[(6.2b) \quad k \mapsto (J(J+1)c_{JLML}(k))_{(J,L) \in \mathbb{Z} \times 1_{L}} \text{ is of class } L^{2}(\mathbb{R}^{+}, \mu; \ell^{2}(Z \times 1_{L})).
\]
Thus \(\text{dom } A_{L} \subseteq \mathcal{H}_{L}\) densely.

The results below imply that \(A_{L}\) is self-adjoint and decomposable. Indeed, let \(P_{L}(k)\) be the projection of \(\mathcal{H}(k)\) onto \(\mathcal{H}_{L}(k)\). Let \(B_{L}(k) := P_{L}(k)A(k)\). Since \(P_{L}(k)\) is orthogonal and \(A(k)\) is self-adjoint, we have \(B_{L}(k)^{*} = A(k)P_{L}(k)\). By
Lemma 6.2 below, $B_L(k)$ is symmetric. Thus $B_L(k) \subseteq B_L(k)^*$. On the other hand, dom $B_L(k)^* \subseteq S_L(k)$; so for $\psi_L(k) \in \text{dom} B_L(k)^*$ and $\phi_L(k) \in S_L(k)$

$$B_L(k)P_L(k)\psi_L(k) = B_L(k)\psi_L(k),$$

$$\langle B_L(k)P_L(k)\psi_L(k), \phi_L(k) \rangle_{S_L(k)} = \langle A(k)P_L(k)\psi_L(k), \phi_L(k) \rangle_{S_L(k)}$$

Thus $B_L(k)^* \subseteq B_L(k)$ and we have that $B_L(k)$ is a self-adjoint operator in $S_L(k)$.

Since the projection $P_L(k)$ commutes with $A(k)$, $S_L(k)$ is a reducing (and hence invariant) subspace for $A(k)$ and we have $B_L(k) = A_L(k)$. To a measurable field $k \mapsto A_L(k)$ of self-adjoint decomposable operators corresponds a self-adjoint decomposable operator $A_L = \int_0^c A_L(k)\mu dk$. Using (5.19), $A$ is the orthogonal sum

$$(6.3) A = \bigoplus_L A_L$$

of self-adjoint decomposable operators (6.1), and the sum over $L$ is understood as a strong limit of partial sums.

Let us define

$$(6.4) U_{\lambda L}(J'\Lambda'J\Lambda k) := (-1)^{J+L}U_{\lambda L}(k)(J'\|Y_\lambda\|J) \begin{bmatrix} J' & \Lambda' & L \\ \Lambda & J & \lambda \end{bmatrix}$$

and

$$(6.5a) \tau(\lambda^n\Lambda') := (-1)^J\sqrt{(n+1)(2\Lambda'+1)(\lambda^{n+1}\Lambda'\|\lambda^n(\Lambda)\lambda)}, \quad n \in \mathbb{N}_0,$$

$$(6.5b) \nu(\lambda^n\Lambda') := -\tau(\lambda^{n-1}\Lambda\Lambda), \quad n \in \mathbb{N}.$$ 

Here $(J'\|Y_\lambda\|J)$ is the reduced matrix element for $\langle w_{J'M'}, Y_\lambda, w_{JM'} \rangle_{L_0}$.  

Remarks 6.1. (1) $(J'\|Y_\lambda\|J) = (-1)^{J+J'}(J'\|Y_\lambda\|J')$, which follows from the Wigner–Eckart theorem. For example, let $L_0 = S^2$ be a unit sphere and $w_J = Y_J$; then

$$(6.6) (J'\|Y_\lambda\|J) = \sqrt{(2\lambda + 1)(2\Lambda + 1)} \begin{bmatrix} J & \lambda & J' \\ 0 & 0 & 0 \end{bmatrix}.$$

The reduced matrix element in (6.6) is nonzero iff the integer $J + \lambda + J'$ is even.

(2) $U_{\lambda L}(J'\Lambda'J\Lambda k) = U_{\lambda L}(J\Lambda J'\Lambda' k)$, which is due to (6.4) and the above remark.

Lemma 6.2. The matrix elements of the angulan operator (4.6) with respect to the field (5.18) of orthonormal bases of $S_L(k)$ are given by

$$(6.7a) [A(k)]_{LM_L,LM_L} = cL(L+1),$$

$$(6.7b) [A(k)]_{JLM_L,J\lambda\Lambda LM_L} = \delta_{n1} \delta_{\lambda\lambda} (-1)^{J} \sqrt{2\lambda + 1} U_{\lambda L}(L0J\lambda k)$$

for $n \in \mathbb{N}$, and

$$(6.7c) [A(k)]_{J'\Lambda'J\Lambda L\lambda LM_L,J\lambda\Lambda LM_L} = \delta_{J',J} \delta_{n,J}(cJ(J+1) + n\omega(k)) + \delta_{\lambda\lambda} U_{\lambda L}(J'\Lambda'J\Lambda k)$$

$$(6.7d) \cdot (\delta_{n',n+1} \tau(\lambda^n\Lambda') + \delta_{n,n'+1} \nu(\lambda^n\Lambda'))$$

for $n, n' \in \mathbb{N}$. 
from which (3.47), for \( n \geq 1 \) follows. This completes the proof of the lemma. \( \square \)
7. Eigenspace of angulon

Let $E$ be an eigenvalue of the angulon operator $A$. According to the decomposition (6.3), $E = E_{LML}$ is an eigenvalue of the part $A_L$ of $A$ in $\mathfrak{H}_L$ for some $L$. Since $A_L$ is decomposable relative to $k \mapsto \mathfrak{H}_L(k)$, $E$ is an eigenvalue of $A_L(k)$ for $\mu$-a.e. $k$.

**Theorem 7.1.** Let $E = E_{LML}$ be the eigenvalue of $A_L$ for some $L$. For $\mu$-a.e. $k$, the coordinates of the eigenvector satisfy (5.20), (6.2), and

$$0 = (cL(L + 1) - E)c_{LML}(k)$$

and

$$0 = \delta_n\delta_{\Lambda}(1)^{\lambda}2\Lambda + 1U_{\Lambda}(J\lambda L0k)c_{LML}(k)$$

$$+ (cJ(J + 1) + n\omega(k) - E)c_{JN\Lambda LML}(k)$$

$$+ \sum_{J'}U_{\Lambda}(J\lambda J'k)[H(n - 2)\tau(J'' - J''')c_{J''N-1\Lambda LML}(k)$$

$$+ \nu(J'' - J''')c_{J''N+1\Lambda LML}(k)$$

(7.1b)

for $n \in \mathbb{N}$. The step function $H(x) = 1$ for $x \geq 0$, and $H(x) = 0$ for $x < 0$.

Let $\Omega_{LML}(k)$ be the set of solutions $(E_{LML}, \psi_{LML}(k) \neq 0)$ satisfying (5.20), (6.2), (7.1). $\Omega_{LML}(k)$ is defined for $\mu$-a.e. $k$ and is called the eigenspace of $A_L$.

**Remark 7.2.** Recall that $n \geq 1$ in (7.1b) is finite, i.e. (7.1b) splits into $N$ equations for some finite $N$. When $n = N$, one puts $c_{J\Lambda N+1\Lambda LML}(k) \equiv 0$ in (7.1b).

When $N = 1$ we have Corollary 7.3; when $N = 2$ and $L = 0$ we have Corollary 7.5.

Let us define

$$\Sigma^{(1)}(z, k) := \sum_{J, \lambda} \frac{(2\lambda + 1)U_{\lambda}(J\lambda L0k)^2}{cJ(J + 1) + \omega(k) - z}$$

(7.2)

for $\mu$-a.e. $k$ and some $z \in C$; i.e. if $O_{\mu}$ is the union of all $\mu$-null sets then

$$z \in \mathbb{C} \setminus \sigma_1,$$

where $\sigma_1 := \{\sigma_1(k) \mid k \in \mathbb{R}^+ \setminus O_{\mu}\}$ and

$$\sigma_1(k) := \{cJ(J + 1) + \omega(k) \mid J \in \mathbb{N}_0\}$$

for $\mu$-a.e. $k$.

In particular, (7.3a) holds for $z < 0$. Note that $\sigma_1$ is the subset of the essential spectrum of $A^0$. Indeed, $A^0$ is viewed as $A$ with $U_{\lambda}(k) \equiv 0$ (all $\lambda$), and in this case Theorem 7.1 says that $cJ(J + 1) + n\omega(k)$ is an eigenvalue of infinite multiplicity of $A^0(k)$ for $\mu$-a.e. $k$. Now, $z \in \sigma_1$ implies $k \in \{k \in \mathbb{R}^+ \setminus O_{\mu} \mid z \in \sigma_1(k)\}$, which means that $z$ is such that $\mu(\{k \in \mathbb{R}^+ \mid z \in \sigma_1(k)\}) > 0$.

When $\omega(k)$ in (7.3) is replaced by $2\omega(k)$, we write $\sigma_2$ instead of $\sigma_1$.

**Corollary 7.3.** For $N = 1$, the eigenvalue $E = E_{LML} \in \mathbb{R} \setminus \sigma_1$ of $A_L$ satisfies

$$E = cL(L + 1) - \Sigma^{(1)}(E, k)$$

(7.4)
for \( \mu \)-a.e. \( k \), and the coordinates satisfy
\[
(7.5) \quad c_{J\lambda \lambda LL} (k) = \left( -1 \right)^{\lambda + 1} \frac{\sqrt{2 \lambda + 1} U_{J\lambda LL} (J\lambda L0k)}{cJ(J+1) + \omega(k) - E} c_{LML} (k)
\]
for \( \mu \)-a.e. \( k \).

Corollary 7.3 corresponds to the case when the many-body quantum state accounts for single bath excitations only [1, 2]. We see that \( E \) is of multiplicity \( 2L + 1 \). The coordinate \( c_{LML} (k) \) is found from the normalization condition.

When two-phonon excitations contribute notably, one solves (7.1) for \( N = 2 \). The simplest example is when \( L = 0 \). To state our results we find it convenient to define
\[
(7.6a) \quad \sigma_* := \left\{ \sigma_*(k) \mid k \in \mathbb{R}^+ \setminus \mathcal{O}_\mu \right\} \text{ with }
(7.6b) \quad \sigma_*(k) := \bigcup_{\lambda \in \mathbb{N}_0} \left\{ z \in \mathbb{C} \setminus \sigma_2 | c\lambda(\lambda + 1) + \omega(k) - z = \epsilon_\lambda(z,k) \right\}
\]
for \( \mu \)-a.e. \( k \), where one puts
\[
(7.7) \quad \epsilon_\lambda(z,k) := 2 \left( -1 \right)^\lambda U_\lambda(k)^2 \frac{(\lambda||Y_\lambda||\lambda)^2}{2 \lambda + 1} \sum_{\lambda} \frac{c\lambda(\lambda + 1) + 2\omega(k) - z}{c\lambda(\lambda + 1) + \omega(k) - z}
\]
for \( \mu \)-a.e. \( k \) and \( z \in \mathbb{C} \setminus \sigma_* \).

Let us further define
\[
(7.8a) \quad \Sigma^{(1,2)}_0 (z,k) := \sum_{\lambda} \frac{U_\lambda(k)^2 (\lambda||Y_\lambda||\lambda)^2}{c\lambda(\lambda + 1) + \omega(k) - z - \epsilon_\lambda(z,k)}, \quad z \in \mathbb{C} \setminus \sigma_*
\]
and
\[
(7.8b) \quad \Sigma^{(2)}_{0} (z,k) := \sum_{\lambda} \frac{U_\lambda(k)^2 \epsilon_\lambda(z,k) (\lambda||Y_\lambda||\lambda)^2}{(c\lambda(\lambda + 1) + \omega(k) - z)(c\lambda(\lambda + 1) + \omega(k) - z - \epsilon_\lambda(z,k))}, \quad z \in \mathbb{C} \setminus \left( \sigma_1 \cup \sigma_2 \cup \sigma_* \right)
\]
for \( \mu \)-a.e. \( k \).

Remark 7.4. Note that, when the reduced matrix element \( (\lambda||Y_\lambda||\lambda) \) is as in (6.6), (7.7) formally coincides with (1.7). We mean "formally", since the exact agreement between (7.7) and (1.7) requires an additional assumption imposed on the probability measure \( \mu \). The same applies to (7.8a) versus the integrand in (1.6).

With the above definitions, our result for \( N = 2 \) is the following.

**Corollary 7.5.** For \( N = 2 \), the eigenvalue \( E = E_{00} \) of \( A_0 \) satisfies
\[
(7.9a) \quad E = - \Sigma^{(1,2)}_0 (E, k), \quad E \in \mathbb{R} \setminus \sigma_*
(7.9b) \quad = - \Sigma^{(1)}_0 (E, k) - \Sigma^{(2)}_{0} (E, k), \quad E \in \mathbb{R} \setminus \left( \sigma_1 \cup \sigma_2 \cup \sigma_* \right)
\]
for \( \mu \)-a.e. \( k \), and the coordinates satisfy
\[
(7.10a) \quad c_{J\lambda \lambda 00} (k) = \frac{(-1)^{\lambda + 1} U_\lambda(k) (\lambda||Y_\lambda||0)^2}{c\lambda(\lambda + 1) + \omega(k) - E - \epsilon_\lambda(E,k)} c_{00}(k),
(7.10b) \quad c_{\lambda\lambda 00} (k) = \frac{(-1)^{\lambda + 1} \sqrt{2} U_\lambda(k) (\lambda||\lambda^2\Delta||\lambda)^2 (\lambda||Y_\lambda||\lambda)}{\sqrt{2} \lambda + 1 (c\lambda(\lambda + 1) + 2\omega(k) - E)} c_{\lambda\lambda 00}(k)
\]
for \( E \in \mathbb{R} \setminus \left( \sigma_2 \cup \sigma_* \right) \) and \( \mu \)-a.e. \( k \).
We close the present section by providing the proofs of the above statements.

Proof of Theorem 7.1. Since $A_L$ is densely defined in $\mathcal{H}_L$, there exists a bounded decomposable $B_L \in \mathcal{B}(\mathcal{H}_L)$ such that $A_L \subseteq B_L$. Hence we have $A_L(k) \subseteq B_L(k)$ for $\mu$-a.e. $k$ (recall e.g. [16, Proposition 12.1.8(i)]), and the matrix elements of $B_L$ with respect to the field (5.18) of orthonormal bases of $\mathcal{H}_L(k)$ are found from Lemma 6.2. Since $\mathcal{B}(\mathcal{H}_L)$ is the strong closure of the finite rank operators, we have

$$B_L(k) = \sum_{i,j} [B_L(k)]_{ij} \langle f_j(k), \gamma \rangle_{\mathcal{H}_L} f_i(k)$$

($\mu$-a.e. $k$), where $[B_L(k)]_{ij}$ is the matrix element of $B_L(k)$ with respect to the orthonormal basis $(f_i(k))$ of $\mathcal{H}_L(k)$; the infinite sum over indices $i,j$ is a strong limit of partial sums. Thus, for $(f_i)$ as in (5.18) and for $\psi_{LM}(k) \in \text{dom} A_L(k)$

$$A_L(k)\psi_{LM}(k) = B_L(k)\psi_{LM}(k)$$

$$= \sum_{j} [A(k)]_{LM,LM} \langle w_{LM} \otimes 1(k), \psi_{LM}(k) \rangle_{\mathcal{H}_L(k)}$$

$\cdot \langle w_{LM} \otimes 1(k), \psi_{LM}(k) \rangle_{\mathcal{H}_L(k)}$

$$+ \sum_{j} \langle A(k)j_L,LM \rangle \langle \psi_{LM}(k) \rangle_{\mathcal{H}_L(k)}$$

$$+ \sum_{j':j'} \langle A(k)j'_{L'},LM \rangle \langle \psi_{LM}(k) \rangle_{\mathcal{H}_L(k)}$$

(7.11)

When $A_L(k)\psi_{LM}(k) = E_{LM} \psi_{LM}(k)$, using (5.20) we thus have (7.1). □

Proof of Corollary 7.3. Put $n = 1$ in (7.1b) and apply $c_{JX_{n}A_{LM}}(k) \equiv 0$ for $n \geq 2$ and $c_{JX_{n}A_{LM}}(k) = \delta_{LM} c_{JX_{n}A_{LM}}(k)$ by (5.20c). □

Proof of Corollary 7.5. First we note that, for $\mu$-a.e. $k$ and $z \in \mathbb{C} \setminus (\sigma_1 \cup \sigma_2 \cup \sigma_*)$, the relation

$$\Sigma_{(1,2)}(z, k) = \Sigma_{(1)}(z, k) + \Sigma_{(2)}(z, k)$$

follows directly from (7.2) with $L = 0$ and (7.8).

When $L = 0$, using $c_{JX_{n}A_{LM}}(k) = \delta_{LM} c_{JX_{n}A_{LM}}(k)$ by (5.20c), relation (7.1b) with $n = 1$ and $n = 2$ reads

$$c_{\lambda \lambda_{1}A_{00}}(k) = \frac{(-1)^{\lambda+1}U_{\lambda}(k)\langle \lambda|Y\rangle|0)}{c\lambda(\lambda + 1) + \omega(k) - E}c_{\lambda \lambda_{2}A_{00}}(k)$$

(7.12a)

$$- \frac{\sqrt{2}U_{\lambda}(k)\Sigma_{\lambda}(\lambda|Y\rangle\lambda)}{2\lambda + 1(c\lambda(\lambda + 1) + \omega(k) - E)}c_{\lambda \lambda_{2}A_{00}}(k)$$

for $E \in \mathbb{R} \setminus \sigma_1$ and $\mu$-a.e. $k$, and

$$c_{\lambda \lambda_{2}A_{00}}(k) = \frac{(-1)^{\lambda+1}\sqrt{2}U_{\lambda}(k)\langle \lambda|Y\rangle\lambda}{2\lambda + 1(c\lambda(\lambda + 1) + 2\omega(k) - E)}c_{\lambda \lambda_{1}A_{00}}(k)$$

for $E \in \mathbb{R} \setminus \sigma_1$ and $\mu$-a.e. $k$, and
\[ (7.12b) \quad (\lambda Y_\lambda \| \lambda^2 \lambda A') \frac{c_{\lambda \lambda^2 \lambda} 0_0(k)}{2\lambda' + 1} \]

for \( E \in \mathbb{R} \setminus \sigma_2 \) and \( \mu \)-a.e. \( k \). Since \( N = 2 \), putting \( c_{\lambda \lambda^2 \lambda} 0_0(k) = 0 \) we deduce (7.10). Relations in (7.9) then follow from (7.1a) and (7.12), since we have for \( L = 0 \)

\[ E_{00}(k) = \sum_\lambda U_\lambda(k) 0(k) c_{\lambda \lambda^2 \lambda} 0_0(k) \]

for \( \mu \)-a.e. \( k \).

\[ \square \]

8. Infimum of the spectrum with a.c. measure

Let \( \Theta_L \) be the numerical range of \( A_L \). Then, \( \Theta_L \) is the set

\[ (8.1) \quad \Theta_L := \{ \mathcal{E}[\psi_{LM_L}] \mid \psi_{LM_L} \in \text{dom} A_L \setminus \{0\} \} \]

of the real numbers

\[ (8.2) \quad \mathcal{E}[\psi_{LM_L}] := \|\psi_{LM_L}\|_S^2 \langle \psi_{LM_L}, A_L \psi_{LM_L} \rangle_s, \quad \psi_{LM_L} \neq 0. \]

Note that \( \psi_{LM_L} \neq 0 \) means that \( \psi_{LM_L}(k) \neq 0 \) for \( \mu \)-a.e. \( k \). One regards \( \mathcal{E}[\cdot] \) as a functional \( \text{dom} A_L \rightarrow \mathbb{R} \) whose value is given by (8.2). We put

\[ (8.3) \quad \mathcal{E} = \mathcal{E}_{LM_L} := \inf \Theta_L \]

provided that \( \mathcal{E}_{LM_L} > -\infty \) exists. By general principles, the spectrum \( \sigma(A_L) \) of \( A_L \) is contained in the closure \( \Theta_L \) and

\[ (8.4) \quad \inf \sigma(A_L) = \mathcal{E}_{LM_L}. \]

Let us further define the functional \( E[\cdot] : \text{dom} A_L \rightarrow \mathbb{R} \) with the value

\[ (8.5) \quad E[\psi_{LM_L}] := \|\psi_{LM_L}\|_S^2 \int E_{LM_L} \|\psi_{LM_L}(k)\|_S^2(k) \mu(dk) \]

for \( (E_{LM_L}, \psi_{LM_L}(k)) \) in the eigenspace \( \Omega_{LM_L}(k) \). We denote by \( \mathcal{E}_L \) the set of all such (8.5).

**Lemma 8.1.** \( \mathcal{E}_{LM_L} = \inf \Theta_L. \)

**Proof.** Let \( \psi_{LM_L} \in \text{dom} A_L \). Using (7.11), the minimization of \( \mathcal{E}[\psi_{LM_L}] \) with respect to \( c_{LM_L}(k) \) and \( c_{LT_{LM_L}}(k) \) leads to (7.1a) and (7.1b), respectively, with

\[ E_{LM_L} = \mathcal{E}[\psi_{LM_L}] \]

for \( \mu \)-a.e. \( k \). Using (8.1), (8.3), and (8.5), we thus have the result as claimed. \( \square \)

**Remark 8.2.** For \( \psi_{LM_L} \) as in (8.5), Theorem 7.1 says that \( \psi_{LM_L} \neq 0 \) implies \( c_{LM_L}(k) \neq 0 \) for \( \mu \)-a.e. \( k \).

The next Theorem 8.3 allows one to estimate \( \mathcal{E} \) for a.c. \( \mu \).

**Theorem 8.3.** Assume that \( \mu \ll dk \), with the Radon–Nikodym derivative supported on \( \mathbb{R}^+ \). Then

\[ (8.6a) \quad \mathcal{E}_{LM_L} = \min\{cL(L + 1) - \Sigma_{LM_L}, cL(L + 1)\}, \quad \text{where} \]

\[ (8.6b) \quad \Sigma_{LM_L} := \sup \int \sum_{\lambda} (-1)^{\lambda + 1} \sqrt{2\lambda + 1} U_{LM}(L0J\lambda k) \frac{c_{LM}(\lambda \lambda \lambda)}{c_{LM}(k)} dk. \]
The supremum is taken over the points of the eigenspace $\Omega_{L,M_L}(k)$ for a.e. $k$, and the coordinates satisfy in addition
\begin{equation}
1 = |c_{L,M_L}(k)|^2 + \sum_{J \Gamma} |c_{J,J',M_L}(k)|^2 \quad \text{for a.e. } k.
\end{equation}

The following Corollaries 8.4 and 8.5 are useful for evaluating the contribution of single-phonon and two-phonon (for $L = 0$) excitations.

**Corollary 8.4.** Assume that $\mu < dk$, with the Radon–Nikodym derivative supported on $\mathbb{R}^+$. Then, $A_L \geq \mathcal{E}$, where the infimum $\mathcal{E} = \mathcal{E}_{L,M_L}$ satisfies
\begin{equation}
\mathcal{E} = \min\{c_L(L + 1) - \Sigma_L^{(1)}(\mathcal{E}) - \Sigma_L^{(2)}(\mathcal{E}), c_L(L + 1)\}, \quad \text{with}
\end{equation}
\begin{equation}
\Sigma_L^{(1)}(\mathcal{E}) := \int \Sigma_L^{(1)}(\mathcal{E}, k)dk, \quad \Sigma_L^{(2)}(\cdot, k) \text{ as in (7.2),}
\end{equation}
provided that the principal value exists, and
\begin{equation}
\Sigma_L^{(1)} := \sup \int \sum_{\lambda, \lambda'} (-1)^{\lambda+1} \sqrt{2(2\lambda + 1)(2\lambda + 1)}(\lambda\lambda|\lambda^2\lambda) \cdot \sum_{J} c_{J,\lambda',M_L}(k) \sum_{J'} c_{J',\lambda,\lambda'}(k) \int \Sigma_L^{(1)}(\mathcal{E}, k)dk, \quad j \in \{1, 2\}
\end{equation}
where $E = E_{L,M_L}$ is the eigenvalue of $A_L$. The supremum is taken over the points of the eigenspace $\Omega_{L,M_L}(k)$ for a.e. $k$, with the coordinates satisfying in addition (8.7).

**Corollary 8.5.** Assume that $\mu < dk$, with the Radon–Nikodym derivative supported on $\mathbb{R}^+$. Then, $A_0 \geq \mathcal{E}$, where the infimum $\mathcal{E} = \mathcal{E}_{00}$ satisfies
\begin{equation}
\mathcal{E} = \min\{-\Sigma_0^{(1)}(\mathcal{E}) - \Sigma_0^{(2)}(\mathcal{E}) - \Sigma_{00}^{''}, 0\}, \quad \text{with}
\end{equation}
\begin{equation}
\Sigma_0^{(j)}(\mathcal{E}) := \int \Sigma_0^{(j)}(\mathcal{E}, k)dk, \quad j \in \{1, 2\}
\end{equation}
provided that the principal value exists, where $\Sigma_0^{(1)}(\cdot, k)$ and $\Sigma_0^{(2)}(\cdot, k)$ are as in (7.2) and (7.8b), and
\begin{equation}
\Sigma_{00}^{''} := \sup \int \sum_{\lambda, \lambda'} (-1)^{\lambda+1} \sqrt{2U_{\lambda}\lambda\lambda^2\lambda}(0)\sqrt{(c\lambda(\lambda + 1) + \omega(k) - \epsilon_0\epsilon_0(E,k))}\cdot \sum_{J} c_{J,\lambda',\lambda_00}(k) \sum_{J'} c_{J',\lambda,\lambda'}(k) \int \Sigma_0^{(1)}(\mathcal{E}, k)dk, \quad j \in \{1, 2\}
\end{equation}
where $E = E_{00}$ is the eigenvalue of $A_0$. The supremum is taken over the points of the eigenspace $\Omega_{00}(k)$ for a.e. $k$, with the coordinates satisfying in addition (8.7) with $L = 0$.

When single-phonon excitations contribute notably ($N = 1$), Corollary 8.4 approximates to
\begin{equation}
\mathcal{E} = c_L(L + 1) - \Sigma_L^{(1)}(\mathcal{E}) \quad \text{for } \Sigma_L^{(1)}(\mathcal{E}) \geq 0.
\end{equation}
In particular, relation (8.10) holds true for $\mathcal{E} < 0$. In this case $\mathcal{E}$ is just $\Sigma_L^{(1)}(\mathcal{E})$. If we further assume (6.6), we see that (8.10) is exactly (1.2), (1.3). That is, Corollary 8.4 reduces to the equation for the energy first obtained in [1] by
minimizing the energy functional based on an expansion in single bath excitations. The coincidence should not be considered as an unexpected result if one recalls the proof of Lemma 8.1.

By contrast, when two-phonon excitations contribute notably \((N = 2)\), Corollary 8.5 approximates to

\[
\begin{align*}
\Sigma_0^{(1,2)}(\mathcal{E}) & = -\Sigma_0^{(1,2)}(\mathcal{E}) \\
\Sigma_0^{(1,2)}(\mathcal{E}) & = -\Sigma_0^{(1)}(\mathcal{E}) - \Sigma_0^{(2)}(\mathcal{E})
\end{align*}
\]

for \(\Sigma_0^{(1,2)}(\mathcal{E}) \geq 0\), where we put

\[
\Sigma_0^{(1,2)}(\mathcal{E}) := \int \Sigma_0^{(1,2)}(\mathcal{E}, k) dk
\]

with \(\Sigma_0^{(1,2)}(\cdot, k)\) as in (7.8a). If we assume (6.6), we see that \(\Sigma_0^{(1,2)}(\mathcal{E})\) is exactly (1.6).

We now close the present section by giving the proofs of Theorem 8.3 and Corollaries 8.4 and 8.5.

**Proof of Theorem 8.3.** Since \(\mu(dk) = \phi(k)dk\), with \(\text{supp } \phi = \mathbb{R}^+\) and \(\phi > 0\) a.e. on \(\mathbb{R}^+\),

\[
|\sigma| = 0 \iff \mu(\sigma) = 0 \quad \text{and hence } |\sigma| > 0 \iff \mu(\sigma) > 0
\]

for \(\sigma \in \mathcal{F}\). Here \(|\cdot|\) is a standard Lebesgue (length) measure. Thus, the relations that hold for \(\mu\)-a.e. \(k\), also hold for a.e. \(k\), and vice versa. In particular, \(E_{L_{LM}}\) is an eigenvalue of \(A_L\) iff \(E_{L_{LM}}\) is an eigenvalue of \(A_L(k)\) for a.e. \(k\). If, further, \(\psi_{L_{LM}}(k)\) is the corresponding eigenvector of \(A_L(k)\) such that \(||\psi_{L_{LM}}||_0 = 1\), then (8.5) coincides with

\[
\begin{align*}
E[\Psi_{L_{LM}}] & := \int E_{L_{LM}}||\Psi_{L_{LM}}(k)||^2_{\mathcal{H}(k)} dk, \quad \text{where} \\
\Psi_{L_{LM}}(k) & := \sqrt{\phi(k)}\psi_{L_{LM}}(k) \quad \text{a.e.}
\end{align*}
\]

The normalization of the vector field \(\psi_{L_{LM}}\) implies (8.7) and

\[
0 < ||\Psi_{L_{LM}}(k)||^2_{\mathcal{H}(k)} < 1 \quad \text{a.e.}
\]

By Theorem 7.1, for a.e. \(k\)

\[
E_{L_{LM}} = c_L(L + 1) - \sum \Psi_{L_{LM}}(k), \quad \text{where}
\]

\[
\sum \Psi_{L_{LM}}(k) := \sum (-1)^{\lambda + 1} \sqrt{2\lambda + 1} U_{\lambda L}(L0J\lambda k) \frac{c_{LM_L}(k)}{c_{LM_L}(k)}
\]

since \(c_{LM_L}(k) \neq 0\) for a.e. \(k\). Substitute the latter in (8.12) and get that

\[
\begin{align*}
E[\Psi_{L_{LM}}] & = c_L(L + 1) - \sum \Psi_{L_{LM}}, \quad \text{where} \\
\sum \Psi_{L_{LM}} & := \int \sum \Psi_{L_{LM}}(k)||\Psi_{L_{LM}}||^2_{\mathcal{H}(k)} dk.
\end{align*}
\]

The closure \(\mathcal{E}_{L}\) consists of real numbers \(r_{L_{LM}}\) such that, for every \(\epsilon > 0\), there exists a \(E[\Psi_{L_{LM}}] \in \mathcal{E}_{L}\) such that \(|r_{L_{LM}} - E[\Psi_{L_{LM}}]| < \epsilon\). Put

\[
\begin{align*}
E_*[\Psi_{L_{LM}}] & := c_L(L + 1) - \sum_* \Psi_{L_{LM}}, \quad \text{where} \\
\sum_* \Psi_{L_{LM}} & := \int \sum \Psi_{L_{LM}}(k) dk.
\end{align*}
\]
It follows from (8.13), (8.14), (8.15) that
\[ cL(L + 1), E_\omega[\Psi_{LM_L}] \in \mathcal{E}_L. \]

Assume that \( \Sigma[\Psi_{LM_L}(k)] > 0 \) a.e. Then \( E[\Psi_{LM_L}] > E_\omega[\Psi_{LM_L}] \) and \( \inf \mathcal{E}_L \) is given by
\[ \inf E_\omega[\Psi_{LM_L}] = cL(L + 1) + \inf(-\Sigma_\omega[\Psi_{LM_L}]) \]
\[ = cL(L + 1) - \Sigma_{LM_L}, \quad \Sigma_{LM_L} := \sup \Sigma_\omega[\Psi_{LM_L}] \]
where the infimum (resp. supremum) is taken over the points of \( \Omega_{LM_L}(k) \) for a.e. \( k \), and with the coordinates satisfying (8.7).

Assume that \( \Sigma[\Psi_{LM_L}(k)] \leq 0 \) a.e. Then \( cL(L + 1) \leq E[\Psi_{LM_L}] \leq E_\omega[\Psi_{LM_L}] \) and hence \( \inf \mathcal{E}_L = cL(L + 1) \). Since \( \inf \mathcal{E}_L \) is unique and \( \inf \mathcal{E}_L = \mathcal{E}_{LM_L} \) by Lemma 8.1, one deduces (8.6). This completes the proof. \( \square \)

**Remark 8.6.** It follows from the above proof that \( \mathcal{E} < cL(L + 1) \) is an exterior point of \( \Theta_L \). In this case \( \mathcal{E} \) is not an eigenvalue of \( A_L \). However, \( \mathcal{E} \) is an eigenvalue of the discontinuous part of \( A_L \), i.e. \( \mathcal{E} \) belongs to the closure of the point spectrum of \( A_L \).

**Proof of Corollary 8.4.** According to (8.4), \( A_L \supseteq \mathcal{E} \), and \( \mathcal{E} \) is found from Theorem 8.3. Thus, using (8.6) and (7.1b) and (7.2)
\[ \Sigma_{LM_L} = \sup \int \Sigma^{(1)}_L(E, k)dk + \Sigma''_{LM_L}. \]
We have the Cauchy principal value because, according to the definition (7.2) and (7.3), we have to exclude the neighborhood of \( k \) such that \( \mathcal{E} \in \sigma_1(k) \) a.e. Now \( E \supseteq \mathcal{E} \) a.e. implies
\[ \sup \int \Sigma^{(1)}_L(E, k)dk = \int \Sigma^{(1)}_L(\mathcal{E}, k)dk \]
and this shows (8.8). \( \square \)

**Proof of Corollary 8.5.** Eliminate \( c_{\lambda^2A_{00}}(k) \) from the system (7.12), then substitute the obtained \( c_{\lambda^3A_{00}}(k) \) in (8.6) with \( L = 0 \), and get that
\[ \Sigma_{00} = \Sigma^{(1)}_0(\mathcal{E}) + \sup \int \Sigma^{(2)}_0(E, k)dk + \Sigma''_{00} \]
where we also use (8.16), since \( E \supseteq \mathcal{E} \) a.e. For the same reason, the second integral on the right equals \( \Sigma^{(2)}_0(\mathcal{E}) \), and we have (8.9). Note that the Cauchy principal value arises because, according to the definition (7.8b), we have to exclude the neighborhoods of the \( k \)'s such that \( \mathcal{E} \in \sigma_1(k) \cup \sigma_2(k) \cup \sigma_\ast(k) \) a.e. \( \square \)

9. **Summary and concluding remarks**

In the present paper our goal was to propose a systematic and self-consistent way of dealing with higher-order phonon excitations induced by the impurity-boson interaction potential. To achieve the goal, we found the direct integral description of angulon most convenient, since in this representation we were able to work independently of the initially unknown occupation numbers of phonon states. Subsequently, the angular momentum algebra were less involved than it seemed to be from the beginning. Our results agree with those obtained from the minimization of energy
functional when the many-body quantum state is based on an expansion in single-phonon excitations. We note that, within the framework of single bath excitations, the variational approach coincides with the Green function formalism, as defined by Feynman diagrams\textsuperscript{2}. This indicates that the variational energy, and hence our obtained infimum of the spectrum, is a "true" lowest energy.

Most challenging tasks arise when one deals with higher-order phonon excitations. Theorems 7.1 and 8.3 allow one to calculate the energies when finitely many phonon excitations are considered. The solutions of equations in Theorem 7.1 seem to be complicated in general, but in special cases they are elegant enough. As an example, we have found that the two-phonon excitations cannot be ignored for a molecule in superfluid $^4$He. When the impurity-bath interaction excites three and more phonons at the same time, one needs in addition the values of the SCFPs as given in Tab. 1; the other values are obtained from the formulas derived in Sec. 5.2.

We believe that the results reported in the paper can be further developed. Of course, finding the solutions of Theorems 7.1 would be enough to accomplish the major part of the task, but there are less complicated, yet physically relevant, pieces of work to do as well. For example, one would like to say more about the spectral parts of the angulon operator, as modeled in the present paper. In this respect the resolvent is of special interest. The analysis of the resolvent allows one to extend the present results of the eigenspace to the entire spectrum, including resonances.

**Acknowledgments**

The author acknowledges productive discussions with Mikhail Lemeshko.

**References**

[1] Richard Schmidt and Mikhail Lemeshko. Rotation of Quantum Impurities in the Presence of a Many-Body Environment. *Phys. Rev. Lett.*, 114:203001, 2015.
[2] Richard Schmidt and Mikhail Lemeshko. Deformation of a Quantum Many-Particle System by a Rotating Impurity. *Phys. Rev. X*, 6:011012, 2016.
[3] Bikashkali Midya, Michal Tomza, Richard Schmidt, and Mikhail Lemeshko. Rotation of Cold Molecular Ions in a Bose–Einstein Condensate. *arXiv:1607.06092*, 2016.
[4] M. Griesemer and A. Wünsch. Self-adjointness and domain of the Fröhlich Hamiltonian. *J. Math. Phys.*, 57:021902, 2016.
[5] J. T. Devreese. Fröhlich Polarons. Lecture course including detailed theoretical derivations. *arXiv:1012.4576v6*, 2015.
[6] J Peter Toennies and Andrey F. Vilesov. Superfluid Helium Droplets: A Uniquely Cold Nanomatrix for Molecules and Molecular Complexes. *Angew. Chem. Int. Ed.*, 43(20):2622–2648, 2004.
[7] M. Lemeshko and R. Schmidt. Molecular impurities interacting with a many-particle environment: from ultracold gases to helium nanodroplets. RSC, 2016.
[8] Jonathan B. Balewski, Alexander T. Krupp, Anita Gaj, David Peter, Hans Peter Buchler, Robert Low, Sebastian Hofferberth, and Tilman Pfau. Coupling a single electron to a Bose–Einstein condensate. *Nature*, 502(7473):664–667, 2013.
[9] Richard Schmidt, H. R. Sadeghpour, and E. Demler. Mesoscopic Rydberg Impurity in an Atomic Quantum Gas. *Phys. Rev. Lett.*, 116:105302, Mar 2016.
[10] W. Töws and G. M. Pastor. Many-Body Theory of Ultrafast Demagnetization and Angular Momentum Transfer in Ferromagnetic Transition Metals. *Phys. Rev. Lett.*, 115:217204, 2015.
[11] Zenonas Rudzikas. *Theoretical Atomic Spectroscopy*. Cambridge University Press, Cambridge, 2 edition, 2007.
[12] Z. Rudzikas and J. Kaniauskas. *Quasispin and Isospin in the Theory of Atom*. Mokslas Publishers, Vilnius, 1984 (in Russian).

\textsuperscript{2}Private communication with M. Lemeshko.
[13] F. A. Berezin. *The Method of Second Quantization*. Academic Press, Inc., London LTD, 2 edition, 1986 (in Russian).
[14] Ola Bratteli and Derek W. Robinson. *Operator Algebras and Quantum Statistical Mechanics: Equilibrium States. Models in Quantum Statistical Mechanics*. Springer-Verlag Berlin Heidelberg, 2 edition, 1997.
[15] Michael Reed and Barry Simon. *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness*. Academic Press, Inc., London LTD, 1975.
[16] Konrad Schmüdgen. *Unbounded Operation Algebras and Representation Theory. Operator Theory: Advances and Applications*, volume 37. Springer Basel AG, 1990.
[17] Jacques Dixmier. *Von Neumann Algebras*. North-Holland Publishing Company, Amsterdam, 1981.
[18] Michael Reed and Barry Simon. *Methods of Modern Mathematical Physics IV: Analysis of Operators*. Academic Press, Inc., London LTD, 1978.
[19] I. B. Frenkel. Two Constructions of Affine Lie Algebra Representations and Boson-Fermion Correspondence in Quantum Field Theory. *J. Funct. Anal.*, 44(3):259–327, 1981.
[20] N. Bourbaki. *Topological Vector Spaces*, volume 1-5. Springer, Springer-Verlag Berlin Heidelberg New York, 2003.
[21] Claude Chevalley. *The Algebraic Theory of Spinors and Clifford Algebras. Collected Works*, volume 2. Springer-Verlag Berlin Heidelberg, 1997.
[22] R. A. Adams and J. J. Fournier. *Sobolev Spaces*. Elsevier Science Ltd, Oxford, UK, 2 edition, 2003.
[23] Christopher Lance. Direct Integrals of Left Hilbert Algebras. *Math. Ann.*, 216:11–28, 1975.
[24] A. U. Klimyk. *Matrix Elements and Clebsch–Gordan Coefficients of Representations of Groups*. Naukova Dumka, Kiev, 1979 (in Russian).
[25] A. P. Jucys and A. A. Bandzaitis. *The Theory of Angular Momentum in Quantum Mechanics*. Mintis Publishers, Vilnius, 2 edition, 1977 (in Russian).
[26] A. P. Jucys, I. B. Levinson, and V. V. Vanagas. *Mathematical Apparatus of the Angular Momentum Theory*. Vilnius, 3 edition, 1960 (in Russian).
[27] A. P. Jucys and A. J. Savukynas. *Mathematical Foundations of the Atomic Theory*. Vilnius, 1973 (in Russian).

VILNIUS UNIVERSITY, INSTITUTE OF THEORETICAL PHYSICS AND ASTRONOMY, SUELÈTEKIO AVE. 3, 10222 VILNIUS, LITHUANIA

E-mail address: Rytis.Jursenas@tfai.vu.lt