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Perturbation Expansion of the Wave Function of Boson Systems

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Abstract. For applications, the Rayleigh-Schrödinger nondegenerate second order perturbation expansion of a many-particle wave-function is explicitly presented. The wave-function represents an assembly of bosons in a perturbing potential. The potential, expressed in second-quantized form, is linear and bilinear in the boson operators and contains arbitrary operators which couple the bosons to other systems of particles.

I. Introduction

In perturbation treatments of boson systems, the perturbing potential usually has the form

$$\hat{V} = \sum_{\boldsymbol{k}\boldsymbol{k}'} \hat{Q}_{\boldsymbol{k}\boldsymbol{k}'}\, \hat{a}_{\boldsymbol{k}}^{\dagger}\, \hat{a}_{\boldsymbol{k}'} + \sum_{\boldsymbol{k}} \hat{Q}'_{\boldsymbol{k}}\, \hat{a}_{\boldsymbol{k}} + \sum_{\boldsymbol{k}} \hat{Q}'^{\dagger}_{\boldsymbol{k}}\, \hat{a}_{\boldsymbol{k}}^{\dagger}\,. \tag{1.1}$$

Here $\hat{a}_{\boldsymbol{k}}$ is the operator which destroys a boson of wave vector [2]) $\boldsymbol{k}$, subject to the usual boson commutation rules. It acts on the unperturbed eigenkets in the occupation number representation. $\hat{Q}_{\boldsymbol{k}\boldsymbol{k}'}$ and $\hat{Q}'_{\boldsymbol{k}}$ are arbitrary operators acting in a space independent of the boson occupation numbers, but may depend on the boson wave vectors and are restricted by the requirement that $\hat{V}$ be Hermitian.

This form of perturbation arises especially often in problems involving crystal lattices, in which case the $\hat{a}$ operators may correspond to phonons or magnons, and the $\hat{Q}$ operators may correspond to phonons or magnons, spins, electrons or localized excitation modes. For example a study of lattice distortions by an impurity [1] would involve local oscillator-phonon interactions, or a study of polarization of magnetic ions in a crystal by an impurity spin [2] would present us with the problem of localized spin-magnon interactions. The treatment of electrical resistivity involves electron-magnon interactions [3, 4] and the theory of magnetoelastic effects [5] deals with magnon-phonon interactions.

A perturbation treatment of this specific form of potential therefore would be useful. We have calculated the wave function for this potential up to and

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[2]) We use the term 'wave vector' to denote the subscript $\boldsymbol{k}$, which enumerates the boson states.

including second-order terms, according to the non-degenerate Rayleigh-Schrödinger perturbation theory [6], assuming the unperturbed Hamiltonian to be of the form

$$\hat{H}_0 = \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} \, \hat{a}_{\boldsymbol{k}}^{\dagger} \, \hat{a}_{\boldsymbol{k}} + \hat{H}' \tag{1.2}$$

where $\varepsilon_{\boldsymbol{k}}$ is the excitation energy of a boson of wave vector $\boldsymbol{k}$ and $\hat{H}'$ is an arbitrary Hermitian operator acting in a space independent of the boson occupation numbers.

II. Perturbation Theory

In general, the perturbed Hamiltonian is written as

$$\hat{H} = \hat{H}_0 + g \, \hat{V} \, , \tag{2.1}$$

where $\hat{H}_0$ is the unperturbed Hamiltonian, $\hat{V}$ is the perturbing potential, and g is the perturbation expansion parameter. The unperturbed eigenvalues and eigenkets obey the equations

$$\hat{H}_0 \, | m \rangle = E_m \, | m \rangle \, , \tag{2.2}$$

and

$$\langle i | m \rangle = \delta_{i m} \, , \tag{2.3}$$

where δ_{im} is the Kronecker symbol. The eigenvector problem to be solved is

$$\hat{H} \, | m) = \mathcal{E}_m \, | m) \, , \tag{2.4}$$

where $\mathcal{E}_m$ and $|m)$ are the perturbed eigenvalues and eigenkets.

According to non-degenerate perturbation theory, we expand the perturbed eigenvalues and eigenkets in powers of g and write

$$| m) = | m \rangle + \sum_{l=1}^{\infty} g^l \, | m)_l \, , \tag{2.5}$$

where $|m)_l$ is given in terms of the unperturbed eigenkets. The Rayleigh-Schrödinger theory yields

$$| m)_1 = \sum_{i \neq m} \frac{\langle i | \hat{V} | m \rangle}{E_m - E_i} \, | i \rangle \, , \tag{2.6}$$

and

$$\begin{aligned} | m)_2 = & - \frac{| m \rangle}{2} \sum_{i \neq m} \frac{|\langle i | \hat{V} | m \rangle|^2}{(E_m - E_i)^2} - \langle m | \, \hat{V} \, | m \rangle \sum_{i \neq m} \frac{\langle i | \hat{V} | m \rangle}{(E_m - E_i)^2} \, | i \rangle \\ & + \sum_{i \neq m} \sum_{j \neq m} \frac{\langle j | \hat{V} | i \rangle \, \langle i | \hat{V} | m \rangle}{(E_m - E_j) \, (E_m - E_i)} \, | j \rangle \, , \end{aligned} \tag{2.7}$$

as the first two terms in Equation (2.5). The $|m)_l$ in Equations (2.6) and (2.7) are so chosen that

$$(i \mid m) = \delta_{i m} + \text{terms of order } g^3 \text{ and higher.} \tag{2.8}$$

An eigenket of $\hat{H}_0$ as given in Equation (1.2) is labelled in the boson occupation number representation by a particular set i of occupation numbers, one for each allowed wave vector, denoted by

$$\{n_{\boldsymbol{k}}^i\} = n_{\boldsymbol{k}_1}^i, n_{\boldsymbol{k}_2}^i, \ldots, n_{\boldsymbol{k}_N}^i \tag{2.9}$$

for N allowed wave vectors. Since each occupation number $n_{\boldsymbol{k}}$ may be an arbitrary integer, there are an infinite number of such sets i. The eigenkets of H' [cf. Equation (1.2)] will be labelled by Greek letters to avoid confusion. Our unperturbed eigenvalue equation is then

$$\hat{H}_0 \,|\alpha\rangle\, |\{n_{\boldsymbol{k}}^i\}\rangle = \Big(E_\alpha + \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}}\, n_{\boldsymbol{k}}^i\Big)\, |\alpha\rangle\, |\{n_{\boldsymbol{k}}^i\}\rangle\,, \tag{2.10}$$

where E_α and $|\alpha\rangle$ are the eigenvalues and eigenkets of $\hat{H}'$.

We see from Equation (2.10) that degeneracies are present in the boson occupation number representation which lead to infinite terms in the sums of Equations (2.6) and (2.7). It is usual to replace these sums by integrals in the limit of infinite systems [$N \to \infty$ in Equation (2.9)]. If these integrals converge, the perturbation expansion remains valid and is approximately correct for large finite systems. In the divergent case, second order Rayleigh-Schrödinger non-degenerate perturbation theory cannot be used.

The matrix elements of $\hat{V}$ [cf. Equation (1.1)] needed in Equations (2.6) and (2.7) are given by:

$$\begin{aligned}
\langle\alpha|\,\langle\{n_{\boldsymbol{k}}^i\}|\, \hat{V}\, |\{n_{\boldsymbol{k}}^j\}\rangle\, |\beta\rangle &= \delta(\{n_{\boldsymbol{k}}^i\}, \{n_{\boldsymbol{k}}^j\}) \sum_{\boldsymbol{k}} n_{\boldsymbol{k}}^j \langle\alpha|\, \hat{Q}_{\boldsymbol{k}\boldsymbol{k}}\, |\beta\rangle \\
&+ \Delta^*(\{n_{\boldsymbol{k}}^i\}, \{n_{\boldsymbol{k}}^j\}) \sum_{\boldsymbol{k}, \boldsymbol{k}'}^{\boldsymbol{k} \neq \boldsymbol{k}'} [(n_{\boldsymbol{k}}^j + 1)\, n_{\boldsymbol{k}}^j]^{1/2} \langle\alpha|\, \hat{Q}_{\boldsymbol{k}\boldsymbol{k}'}\, |\beta\rangle\, \delta(n_{\boldsymbol{k}}^i, n_{\boldsymbol{k}}^j + 1)\, \delta\,(n_{\boldsymbol{k}'}^i, n_{\boldsymbol{k}'}^j - 1) \\
&+ \Delta(\{n_{\boldsymbol{k}}^i\}, \{n_{\boldsymbol{k}}^j\}) \sum_{\boldsymbol{k}} [(n_{\boldsymbol{k}}^j)^{1/2} \langle\alpha|\, \hat{Q}'_{\boldsymbol{k}}\, |\beta\rangle\, \delta\,(n_{\boldsymbol{k}}^i, n_{\boldsymbol{k}}^j - 1) \\
&+ (n_{\boldsymbol{k}}^j + 1)^{1/2} \langle\alpha|\, \hat{Q}_{\boldsymbol{k}}^{\prime\dagger}\, |\beta\rangle\, \delta\,(n_{\boldsymbol{k}}^i, n_{\boldsymbol{k}}^j + 1)]\,,
\end{aligned} \tag{2.11}$$

where $\delta(a, b)$ is the Kronecker delta of a and b, $\{n_{\boldsymbol{k}}^i\} = \{n_{\boldsymbol{k}}^j\}$ means $n_{\boldsymbol{k}1}^i = n_{\boldsymbol{k}1}^j$, $n_{\boldsymbol{k}2}^i = n_{\boldsymbol{k}2}^j, \ldots, n_{\boldsymbol{k}N}^i = n_{\boldsymbol{k}N}^j$, and Δ and Δ^* are defined as

$$\Delta(\{n_{\boldsymbol{k}}^i\}, \{n_{\boldsymbol{k}}^j\}) = \begin{cases} 1, \text{ if } \{n_{\boldsymbol{k}}^i\} \text{ and } \{n_{\boldsymbol{k}}^j\} \text{ differ at one and only one wave vector} \\ 0, \text{ otherwise} \end{cases} \tag{2.12}$$

and

$$\Delta^*(\{n_{\boldsymbol{k}}^i\}, \{n_{\boldsymbol{k}}^j\}) = \begin{cases} 1, \text{ if } \{n_{\boldsymbol{k}}^i\} \text{ and } \{n_{\boldsymbol{k}}^j\} \text{ differ at two and only two wave vectors} \\ 0, \text{ otherwise} \end{cases} \tag{2.13}$$

III. Perturbed Wave Function

From the results of Section II, the perturbed wave function can now be calculated. But first we describe a few notational conveniences to be used in this section. We suppress the wave vector $\boldsymbol{k}_l$, replacing it by its index l, with sums over l being understood to means sums over all allowed wave vectors $\boldsymbol{k}_l$. From Equations (2.6), (2.7) and (2.11), we see that the unperturbed boson eigenkets will differ by at most a few excitations from the boson occupation numbers of the perturbed eigenket being calculated. If this set is, say, $\{n^i_{\boldsymbol{k}}\}$, we relabel it as 0, remembering of course what the actual occupation numbers are when operating on the kets.

Hence

$$|n^i_1, n^i_2, \ldots, n^i_j, \ldots, n^i_N\rangle \equiv |0, \ldots, 0\rangle . \tag{3.1}$$

Deviations from this set are denoted as

$$\begin{aligned}|n^i_1, n^i_2, \ldots, n^i_j + p, \ldots, n^i_l + q, \ldots, n^i_m + r, \ldots, n^i_N\rangle \\ \equiv |0 \ldots 0, p_j, 0 \ldots 0, q_l, 0 \ldots 0, r_m, 0 \ldots 0\rangle ,\end{aligned} \tag{3.2}$$

and the notation on the left hand side of Equation (3.2) will be replaced by that on the right. The numbers labelling the kets in our new notation will be referred to as 'occupation deviation numbers'.

Although Equation (3.2) has no meaning if any of the wave vectors in the ket are made equal, much simplification will result in the wave function formula if we allow indices to become equal in our new notation and if we define such cases by the convention

$$|0 \ldots 0, p_j, 0 \ldots 0, q_j, 0 \ldots 0, r_m, 0 \ldots 0\rangle , \equiv | \ldots, (p+q)_j, \ldots, r_m, \ldots\rangle . \tag{3.3}$$

Thus the state $|1_{\boldsymbol{k}}, -1_{\boldsymbol{k}}\rangle$ is defined as $|0\rangle$, the original state as given by Equation (3.1), for example. We further subdivide the perturbed eigenket into the parts

$$|\alpha, 0)_1 = |\alpha, 0)^Q_1 + |\alpha, 0)^{Q'}_2 + \text{'conjugate' term}, \tag{3.4}$$

and

$$\begin{aligned}|\alpha, 0)_2 = |\alpha, 0)^{QQ}_2 + |\alpha, 0)^{Q'Q'}_2 + |\alpha, 0)^{QQ'}_2 + |\alpha, 0)^{Q'Q}_2 + |\alpha, 0)^{Q'\dagger Q'}_2 \\ + \text{'conjugate' terms},\end{aligned} \tag{3.5}$$

where α denotes an $\hat{H}'$ eigenstate and 0 denotes any boson eigenstate, as described in Equation (3.1). The subscripts are those of Equations (2.5), (2.6) and (2.7), and the superscripts indicate the operators appearing in the matrix elements of $\hat{V}$ as described by Equations (2.6), (2.7) and (2.11). To each term appearing in Equations (3.4) and (3.5) which contains a $\hat{Q}'$ or $\hat{Q}'^\dagger$ operator, there corresponds a 'conjugate' term in which $\hat{Q}'$ is replaced by $\hat{Q}'^\dagger$ and $\hat{Q}'^\dagger$ is replaced by $\hat{Q}'$. All such terms must be added to Equations (3.4) and (3.5) to obtain the complete perturbed wave function. These terms are not given here explicitly, since they may be derived from their corresponding terms by the following simple set of rules, which will become clear upon examining the terms in the wave function below.

1. Change the sign of each ε having the same subscript as a $\hat{Q}'$ or $\hat{Q}'^\dagger$ operator.
2. Change the sign of each ket boson 'occupation deviation number' having the same subscript as a $\hat{Q}'$ or $\hat{Q}'^\dagger$ operator.

3. Add 1 to each n having the same subscript as a $\hat{Q}'$ operator.
4. Subtract 1 from each n having the same subscript as a $\hat{Q}'^\dagger$ operator.
5. Change the sign of each Kronecker symbol marked with an asterisk.
6. Replace $\hat{Q}'$ by $\hat{Q}'^\dagger$ and $\hat{Q}'^\dagger$ by $\hat{Q}'$ after completing steps 1 through 5.

Each 'conjugate' term is derived by applying all six steps above to its corresponding term as given by Equation (3.7), (3.9), (3.10), (3.11) or (3.12).

The asterisk mark on certain Kronecker deltas below has no other significance than that mentioned in rule 5. Roman letter subscripts below are boson wave vector indices and Greek letters denote eigenstates of H'. The first order terms are

$$|\alpha, 0)_1^Q = \sum_{ij} [(n_i + 1 - \delta_{ij})\, n_j]^{1/2} \sum_\beta{}' \frac{\langle\beta|\hat{Q}_{ij}|\alpha\rangle}{E_\alpha - E_\beta + \varepsilon_j - \varepsilon_i} |\beta\rangle\, |1_i, -1_j\rangle \tag{3.6}$$

and

$$|\alpha, 0)_1^{Q'} = \sum_i n_i^{1/2} \sum_\beta \frac{\langle\beta|\hat{Q}'_i|\alpha\rangle}{E_\alpha - E_\beta + \varepsilon_i} |\beta\rangle\, |-1_i\rangle\,. \tag{3.7}$$

Here and below, the prime on the summation indicates that terms for which the denominator is zero because of equal indices (i.e., not due to degeneracy) are excluded. In this case, $\beta \neq \alpha$ when $i = j$. The first second order term is given by

$$\begin{aligned}
|\alpha, 0)_2^{QQ} = {} & \frac{-|\alpha\rangle\, |0\rangle}{2} \sum_{ij} (n_i + 1 - \delta_{ij})\, n_j \sum_\beta{}' \frac{|\langle\beta|\hat{Q}_{ij}|\alpha\rangle|^2}{(E_\alpha - E_\beta + \varepsilon_j - \varepsilon_i)^2} \\
& - \Big[\sum_i n_i \langle\alpha|\,\hat{Q}_{ii}\,|\alpha\rangle\Big] \sum_{ij} [(n_i + 1 - \delta_{ij})\, n_j]^{1/2} \sum_\beta{}' \frac{\langle\beta|\hat{Q}_{ij}|\alpha\rangle}{(E_\alpha - E_\beta + \varepsilon_j - \varepsilon_i)^2} |\beta\rangle\, |1_i, -1_j\rangle \\
& + \sum_{ijlm} [(n_i + 1 - \delta_{ij})\, n_j\, (n_l + 1 + \delta_{li} - \delta_{lj} - \delta_{lm})\, (n_m + \delta_{mi} - \delta_{mj})]^{1/2} \\
& \times \sum_{\beta\gamma}{}' \frac{\langle\gamma|\hat{Q}_{lm}|\beta\rangle\, \langle\beta|\hat{Q}_{ij}|\alpha\rangle}{(E_\alpha - E_\gamma + \varepsilon_j - \varepsilon_i + \varepsilon_m - \varepsilon_l)\, (E_\alpha - E_\beta + \varepsilon_j - \varepsilon_i)} |\gamma\rangle\, |1_i, -1_j, 1_l, -1_m\rangle\,.
\end{aligned} \tag{3.8}$$

The prime on the double sum above implies that $\beta \neq \alpha$ if $i = j$, and $\gamma \neq \alpha$ if $i = j$ and $l = m$ or if $l = j$ and $m = i$. The remaining second order terms are

$$\begin{aligned}
|\alpha, 0)_2^{Q'Q'} = {} & -\frac{|\alpha\rangle\, |0\rangle}{2} \sum_i n_i \sum_\beta \frac{|\langle\beta|\hat{Q}'_i|\alpha\rangle|^2}{(E_\alpha - E_\beta + \varepsilon_i)^2} \\
& + \sum_{ij} [n_i\, (n_j - \delta^*_{ji})]^{1/2} \sum_{\beta\gamma} \frac{\langle\gamma|\hat{Q}'_j|\beta\rangle\, \langle\beta|\hat{Q}'_i|\alpha\rangle}{(E_\alpha - E_\gamma + \varepsilon_i + \varepsilon_j)\, (E_\alpha - E_\beta + \varepsilon_i)} |\gamma\rangle\, |-1_i, -1_j\rangle\,,
\end{aligned} \tag{3.9}$$

$$\begin{aligned}
|\alpha, 0)_2^{QQ'} = {} & -\Big[\sum_i n_i \langle\alpha|\,\hat{Q}_{ii}\,|\alpha\rangle\Big] \sum_i n_i^{1/2} \sum_\beta \frac{\langle\beta|\hat{Q}'_i|\alpha\rangle}{(E_\alpha - E_\beta + \varepsilon_i)^2} |\beta\rangle\, |-1_i\rangle \\
& + \sum_{ijl} [n_i\, (n_j + 1 - \delta^*_{ji} - \delta_{jl})\, (n_l - \delta^*_{li})]^{1/2} \sum_{\beta\gamma} \frac{\langle\gamma|\hat{Q}_{jl}|\beta\rangle\, \langle\beta|\hat{Q}'_i|\alpha\rangle}{(E_\alpha - E_\gamma + \varepsilon_i + \varepsilon_l - \varepsilon_j)\, (E_\alpha - E_\beta + \varepsilon_i)} \\
& \times |\gamma\rangle\, |-1_i, 1_j, -1_l\rangle\,,
\end{aligned} \tag{3.10}$$

$$|\alpha, 0)_2^{Q'Q} = \sum_{ijl} [(n_i + 1 - \delta_{ij})\, n_j\, (n_l + \delta_{li} - \delta_{lj})]^{1/2}$$

$$\times \sum_{\beta\gamma}{}' \frac{\langle\gamma|\hat{Q}'_l|\beta\rangle \langle\beta|\hat{Q}_{ij}|\alpha\rangle}{(E_\alpha - E_\gamma + \varepsilon_j - \varepsilon_i + \varepsilon_l)\,(E_\alpha - E_\beta + \varepsilon_j - \varepsilon_i)}\, |\alpha\rangle\, |1_i, -1_j, -1_l\rangle\,, \tag{3.11}$$

where the prime on the sum implies that $\beta \neq \alpha$ if $j = i$, and

$$|\alpha, 0)_2^{Q'\dagger Q'} = \sum_i [n_i\, (n_j + 1 - \delta^*_{ji})]^{1/2} \sum_{\beta\gamma}{}' \frac{\langle\gamma|\hat{Q}'^{\dagger}_j|\beta\rangle \langle\beta|\hat{Q}'_i|\alpha\rangle}{(E_\alpha - E_\gamma + \varepsilon_i - \varepsilon_j)\,(E_\alpha - E_\beta + \varepsilon_i)}$$

$$\times\, |\gamma\rangle\, |-1_i, 1_j\rangle\,, \tag{3.12}$$

where the prime on the sum implies that $\gamma \neq \alpha$ if $j = i$. Equations (3.4) through (3.12), when substituted into Equation (2.5), constitute the perturbed wave function of the boson system, correct to second order.

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