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Convergence of the Method of Moments*

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A proof is given that the nth approximation of the method of moments is convergent when applied to the polaron problem.

I. INTRODUCTION

IN an earlier paper the application of the method of moments to the polaron problem was considered.[1] Two empirical facts were observed that suggested that the method was convergent for this problem. It is the purpose of the present work to give a rigorous proof of the convergence. This proof is composed of two elements. The first is a theorem that gives an upper bound on the rate of increase of the moments in order that they be in a one-to-one relationship with a distribution function.[2] Secondly an estimate is made of the moments of the polaron problem. From the nature of the proof it is clear that the method of moments will also be convergent for a wide class of problems.

II. ESTIMATE OF THE POLARON MOMENTS

The estimate of the polaron moment to be made is the crudest one possible. That is, all integrals are estimated by the maximum value of the integrand times the volume of the domain of integration, and all sums are estimated by the largest term times the number of terms.

The moment H_n is the sum of the vacuum expectation values of the 3^n possible permutations of A, B^+, and B^- taken n at a time. (The notation is the same as I.) The nonvanishing terms in this sum may be grouped according to the number s of pairs B^+B^-.

For any value of s the term $(B^-)^s A^{n-2s}(B^+)^s$ is the largest. Consider first the effect of replacing the term B^+A in some matrix element by AB^+. The commutator $[A,B^+]$ is easily evaluated and is given by

$$[A,B^+]=\omega+\frac{-2(\mathbf{p}-\mathbf{k}_1-\mathbf{k}_2-\cdots-\mathbf{k}_r)\cdot\mathbf{k}_{r+1}+\mathbf{k}_{r+1}^2}{2m}.$$

The wave vectors of the phonons in the field are $\mathbf{k}_1$ to $\mathbf{k}_r$, and the interaction B^+ creates the $(r+1)$st phonon. The B^+B^- pairs contribute factors $\int d^3k|V_k|^2$ to the integrals defining the polaron moments, while the A's contribute factors of the forms ω, $\mathbf{p}^2$, $(-\mathbf{p}\cdot\mathbf{k}_i)$, $\mathbf{k}_i\cdot\mathbf{k}_j$, and $\mathbf{k}_i^2$. The commutator thus supplies factors which are not different from those supplied by the A's including the signs. On general grounds of invariance, only expressions that are quadratic in each of the $\mathbf{k}_i$ and $\mathbf{p}$ survive the angular integrations. That this is true may also be seen directly by integrating the expression

$$\int\prod_{i=1}^{n}d\Omega_i\prod_{i\leqslant j=1}^{n}(\mathbf{e}_i\cdot\mathbf{e}_j)^{\alpha_{ij}},$$

where the $\mathbf{e}_i$ are unit vectors. It is also true that the numerical factors that result from this integral are all positive. Thus, the integrals defining the polaron moments have the property that if the integrands are expanded into a sum of monomials and the integration performed termwise, each term in the sum is positive. As the monomials originating from the commutator are identical with those that occur naturally, it follows that the integrals containing the commutator are positive and that the matrix elements containing AB^+ are larger than the corresponding ones containing B^+A.

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[1] F. R. Halpern, Phys. Rev. **109**, 1836 (1958). Referred to as I.

[2] T. Carleman, *Les Fonctions Quasi Analytique* (Gauthier Villars, Paris, 1926), p. 80.

In the same way interchanging the factors B^+B^- leads to an increased matrix element. These two results suffice to construct a chain of ascending inequalities leading from an arbitrary term containing s pairs B^+B^- to the term $(B^-)^s A^{n-2s}(B^+)^s$. Since there are certainly less than 3^n terms containing s pairs, the following inequality holds:

$$H_n \leq 3^n \sum_{s=0}^{[\frac{1}{2}n]} \langle \phi | (B^-)^s A^{n-2s} (B)^s | \phi \rangle.$$

It is now necessary to evaluate the matrix element above. The integral for this matrix element is

$$\int \prod_{i=1}^{n} d^3k_i |V_{k_i}|^2 \left[\frac{(\mathbf{p}-\mathbf{k}_1-\cdots-\mathbf{k}_s)^2}{2m} + s\omega \right]^{n-2s}.$$

There are $s!$ possible permutations of the $\mathbf{k}$'s corresponding to the different orders in which the s phonons are created or destroyed. All these permutations contribute equally to the matrix element. Consequently, only one needs to be evaluated and multiplied by $s!$. The maximum value of the integrand occurs when all s vectors line up and have their maximum value the cutoff K. If the integrand is replaced by this value, an upper bound for the integral is

$$\left[\frac{(p+sK)^2}{2m} + s\omega \right]^{n-2s} \int \prod_{i=1}^{n} d^3K_i |V_{k_i}|^2.$$

The remaining integral is easily evaluated and the result is

$$\left[\frac{(p+sK)^2}{2m} + s\omega \right]^{n-2s} \left(\frac{2\alpha K}{\pi} \right)^s.$$

If this estimate for the integral is substituted into the upper bound derived above for the polaron moment, it becomes

$$H_n \leq 3^n \sum_{s=0}^{[\frac{1}{2}n]} s! \left(\frac{2\alpha k}{\pi} \right)^s \left[\frac{(p+sK)^2}{2m} + s\omega \right]^{n-2s}.$$

For sufficiently large n there exists a constant C such that

$$\frac{(p+sK)^2}{2m} + s\omega < Cn^2.$$

The factor $(2\alpha K/\pi)^s$ is either less than 1 or $(2\alpha K/\pi)^n$; in both cases it may be grouped with the factor 3^n and the combination is less than D^n. With these simplifications, the inequality becomes

$$H_n \leq D^n \sum_{s=0}^{[\frac{1}{2}n]} s! (Cn^2)^{n-2s}$$

$$\leq (CD)^n n^{2n} \sum_{s=0}^{[\frac{1}{2}n]} \left(\frac{s}{n^4} \right)^s \leq (DC)^n n^{2n+1}.$$

Stirling's formula has been used and some trivial redefinitions of C. The final form of the inequality is

$$H_n < C^n n^{2n+1}.$$

III. PROOF OF CONVERGENCE

Carleman's theorem[2] states that if the sum

$$(1/H_n)^{1/(2n)}$$

is divergent, then there is a unique distribution function $F_\phi(E)$ to which the moments belong. The estimate made above of the polaron moment leads to a divergent series and hence there is a unique distribution that generates the polaron moments.

It remains to show that the approximating sequence of functions $F_\phi{}^n(E)$ converge. First consider the points of increase of the approximate functions. They are the roots of the orthogonal polynomials. The ith roots form a decreasing sequence with respect to the index n. Since they are bounded from below, the sequence is convergent. Similarly, the magnitudes of the jumps at the points of discontinuity are monotonic functions of n and hence approach limits. The function $F_\phi{}^n(E)$ is convergent, and from Carleman's theorem it converges to the correct distribution $F_\phi(E)$.

IV. DISCUSSION

The proof of convergence is determined by three considerations: first the cutoff which limits the momentum transfer in elementary interactions, secondly the quadratic dependence of the energy on the momentum, and finally the relatively small number of contributions to each moment. Since only the first condition is artificial, it appears that the present proof may be readily generalized to many physical systems.

In the discussion of the polaron problem,[1] it was suggested that if the method of moments was convergent, then the perturbation series probably is not. The statement was based on the observation that the method of moments generated a sequence $E_n(\alpha)$ of nonanalytic functions of α that converged to the correct ground-state energy $E(\alpha)$. However, it is quite possible to have a sequence of nonanalytic functions converge to an analytic one: consider, for example, $E_n(\alpha) = E(\alpha) + \alpha^{\frac{1}{2}}/n$.[3]

[3] The author would like to thank H. Araki for this remark.