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Abstract

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MATHEMATICAL PHYSICS

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A TRACE FORMULA FOR THE MANY-PARTICLE SCHRÖDINGER EQUATION

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In 1937, Beth and Uhlenbeck established a formula expressing $\mathrm{sp}(e^{-\beta H} - e^{-\beta H_0})$, where $H_0 = -d^2/dx^2$, $H = -d^2/dx^2 + v(x)$, in terms of scattering phases ($v(x)$ is assumed to be a sufficiently rapidly decreasing function) (see (1), pp. 254-257). Subsequently this result was generalized (2), and the resulting expression of the trace in terms of the scattering operator received the name of trace formula. In the present paper trace formulas are established for the many-particle Schrödinger equation. These formulas are closely connected with quantum statistics and are different for different statistics.

1. The Boltzmann case. Consider, in three-dimensional space, a cube A of volume V. Denote by $L_2(n, A)$ the Hilbert space of functions of n variables, each of which ranges over the cube A. In $L_2(n, A)$ consider the operator H_n:

$$H_n = -\sum_1^n \Delta_k + g \sum_{1\le i<j\le n} v(x_i - x_j), \qquad x_k = (x_k^{(1)}, x_k^{(2)}, x_k^{(3)}), \tag{1}$$

where Δ_k is the Laplace operator in the variables x_k. Periodic boundary conditions are meant; g is a real parameter introduced for convenience.

The **Boltzmann statsum** is the series

$$\Xi = 1 + \sum_1^\infty \frac{\xi^n}{n!}\,\mathrm{sp}\, e^{-\beta H_n}. \tag{2}$$

The parameter ξ is called the **activity**. Denote by b_n the coefficient in the expansion of $\frac{1}{V}\ln \Xi$ in powers of ξ. It is not hard to verify that

$$b_n(V) = \frac{1}{V} \sum_{n_1+2n_2+\cdots=n} (-1)^{n_1+n_2+\cdots-1} \frac{(n_1+n_2+\cdots-1)!}{n_1!\,n_2!\cdots(1!)^{n_1}(2!)^{n_2}\cdots} Z_1^{n_1} Z_2^{n_2}\cdots, \tag{3}$$

where $Z_k = \mathrm{sp}\exp(-\beta H_k)$.

Partition the set of n elements into nonintersecting subsets $\Lambda_1, \Lambda_2, \ldots$. In what follows, sums over all such partitions are often encountered. We agree to denote by Λ the partition itself and by $n_k = n_k(\Lambda)$ the number of subsets containing k elements. Thus, $\sum k n_k = n$. Obviously, the number of different partitions with one and the same set of numbers n_k is $n!(n_1!\, n_2! \cdots (1!)^{n_1} (2!)^{n_2} \cdots)^{-1}$. With each partition associate the operator H_Λ, equal to

$$H_\Lambda = -\sum \Delta_k + g \sum_p \sum_{\substack{i<j \\ i,j \in \Lambda_p}} v(x_i - x_j); \tag{4}$$

Λ_p ranges over the collection of subsets entering the partition Λ.

It is obvious that the operator (4) is an operator with separated variables and that

$$\operatorname{sp} \exp(-\beta H_\Lambda) = \big(\operatorname{sp} \exp(-\beta H_1)\big)^{n_1} \big(\operatorname{sp} \exp(-\beta H_2)\big)^{n_2} \cdots . \tag{5}$$

Taking (5) into account, we obtain for $b_n(V)$ the expression

$$b_n(V) = \frac{1}{n!\, V} \operatorname{sp} \left\{ \sum_\Lambda (-1)^{n_1+n_2+\cdots-1} (n_1 + n_2 + \cdots - 1)!\, e^{-\beta H_\Lambda} \right\}. \tag{6}$$

Along with $b_n(V)$, consider the expression

$$\tilde{b}_n(V) = \frac{1}{n! V} \operatorname{sp} \left\{ \sum_\Lambda (-1)^{n_1+n_2+\cdots-1} (n_1 + n_2 + \cdots - 1)!\, F(H_\Lambda) \right\}, \tag{6'}$$

where F is some function.

If F is a function analytic in a neighborhood of the real axis and H is a self-adjoint operator, then

$$F(H) = -\frac{1}{2\pi i} \int F(z)(z - H)^{-1}\, dz.$$

(The integral is taken over a contour enclosing the spectrum of H; the contour is traversed clockwise.) Taking this into account, after simple transformations we obtain for $\tilde{b}_n(V)$, for $n > 1$, the expression

$$b_n(V) = \frac{-1}{2\pi i \cdot n! \cdot V} \times$$

$$\times \operatorname{sp} \int F(z) \frac{d}{dz} \sum_{\Lambda} (-1)^{n_1+\dots-1} (n_1 + \dots - 1)! \ln \left(1 - (z - H_n^{(0)})^{-1} V_\Lambda\right) dz, \quad (7)$$

where $H_n^{(0)}$ denotes the operator $H_n^{(0)} = -\sum \Delta_k$, $V_\Lambda = H_\Lambda - H_n^{(0)}$. In expression (7) it is possible to pass to the limit as $V \to \infty$.* The operator under the trace sign in (7) will be denoted by T_V. As $V \to \infty$, T_V tends to a limit, which we denote by T. After the Fourier transform the operator T is given by a kernel of the form

$$K(p_1 \dots p_n \mid q_1 \dots q_n)\, \delta(p_1 + \dots + p_n - q_1 \cdots q_n), \quad p_i = (p_i^{(1)}, p_i^{(2)}, p_i^{(3)}). \quad (8)$$

The **regularized trace** of the operator given by a kernel of the form (8) will mean the expression

$$\operatorname{sp}_1 T = \int K(p_1 \dots p_n \mid p_1 \dots p_n)\, d^{3n} p. \quad (9)$$

Theorem 1. Let $v(x)$ satisfy the estimate $\int |v(x)|\, d^3 x < \infty$, and let $F(E)$ be a function analytic in a neighborhood of the real axis and satisfying the estimate

$$\int_0^\infty |F(E + i\alpha)| E^{3n-1}\, dE < \infty.$$

Then there exists the limit $\tilde{b}_n = \lim_{V\to\infty} \tilde{b}_n(V)$, which is equal to

$$\tilde{b}_n = \frac{-1}{2\pi i \cdot n!} \times$$

$$\times \operatorname{sp}_1 \int F(z) \frac{d}{dz} \sum_{\Lambda} (-1)^{n_1+n_2+\dots-1} (n_1+n_2+\dots-1)! \ln \left(1 - (z - H_n^{(0)})^{-1} V_\Lambda\right) dz. \quad (10)$$

The sum is extended over all partitions Λ of a set of n elements into disjoint subsets; n_k is the number of subsets containing k elements.

The operator under the trace sign has the form (8), and therefore has no trace in the ordinary sense. It is not hard to verify, however, that it leaves invariant the set of functions of the form $f(p_1, \dots, p_n)\delta(p_1 + \dots + p_n)$. If on this set one introduces the scalar product by the formula

$$(f, f) = \int |f|^2 \delta(p_1 + \dots + p_n)\, d^{3n} p,$$

then one obtains the Hilbert space $L_2^0(n)$. If the function $v(x)$ decreases sufficiently rapidly, then the operator under the trace sign in (10) has in $L_2^0(n)$ a trace in the ordinary sense. The coefficient $\tilde{b}_n$ is easily expressed through the trace of this operator in $L_2^0(n)$.

Consider n points, some of which are joined by lines. The resulting complex will be called **filled** if, together with every closed polygon whose boundary has no self-intersections, it contains all diagonals of this polygon. The number n will be called the **order** of the complex. A complex of order n will be called monolithic if it consists of an n-gon and all its diagonals. It is obvious that every connected filled complex of order n consists of several monolithic complexes of smaller order, and any two of these monolithic complexes either have no common vertices or have exactly one common vertex. We shall call these monolithic subcomplexes the **components of the original complex**. Every filled complex is completely determined by its components. Therefore a complex of k components is naturally denoted by $M = \{M_1, \dots, M_n\}$, where M_k is the set of vertices of the k-th component.

Let us pass to the expression of the coefficient $\tilde{b}_n$ in terms of scattering operators. We denote by S_Λ the scattering operator corresponding to H_Λ. We shall assume that the scattering is purely elastic.* In this case the scattering operator is a unitary operator commuting with $H_n^{(0)}$.** The logarithm S_Λ is a skew-Hermitian operator which, after the Fourier transform, is specified by a kernel of the form

$$2\pi i \delta\left(p_1^2 + \dots + p_n^2 - q_1^2 - \dots - q_n^2\right) \delta(p_1 + \dots + p_n - q_1 - \dots - q_n)\, \sigma_\Lambda(p_1 \dots p_n \mid q_1 \dots q_n), \tag{11}$$

where

$$p_i^2 = \left(p_i^{(1)}\right)^2 + \left(p_i^{(2)}\right)^2 + \left(p_i^{(3)}\right)^2 .$$

To every monolithic complex of order n, whose vertices form the set M, we assign the function

$$E_M(p_{i_1} \dots p_{i_n}) = \sigma(p_{i_1} \dots p_{i_n} \mid p_{i_1} \dots p_{i_n}),$$

where $M = \{i_1, \dots, i_n\}$ is the set of vertices of the complex,

$$\sigma(p_1 \dots p_n \mid q_1 \dots q_n) =$$

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* The existence of the limit $b_n = \lim_{V \to \infty} b_n(V)$ was first established in the work of Lee and Yang (^{3}).

$$= \sum_{\Lambda} (-1)^{n_1+n_2+\dots-1}(n_1+n_2+\dots-1)!\, \sigma_\Lambda(p_1 \dots p_n \mid q_1 \dots q_n). \qquad (12)$$

(The sum extends over all partitions Λ of the set of n elements into nonintersecting subsets; n_k is the number of subsets consisting of k elements.)

Theorem 2. Let $v(x)$ be a finite function and let $F(E)$ be a function defined for $E \geq 0$ and satisfying, together with its first n derivatives, the estimate

$$\int_0^\infty \left|F^{(k)}(E)\right| E^{3n-1}\, dE < \infty.$$

Then there exists the limit $\tilde{b}_n = \lim_{V\to\infty} \tilde{b}_n(V)$, which is equal to

$$\tilde{b}_n = \sum_M \int F^{(k)}(p_1^2 + \dots + p_n^2)\, E_{M_1} \cdots E_{M_k}\, d^{3n}p. \qquad (13)$$

The sum extends over all connected filled complexes of order n, $M = \{M_1, \dots, M_k\}$. The number of the derivative of the function F in the summand corresponding to the complex M is equal to the number of components of the complex.

2. Bose case. The statistical sum in this case is the series

$$\Xi = 1 + \sum_1^\infty \xi^n \operatorname{sp} P_n e^{-\beta H_n}, \qquad (14)$$

where P_n is the projection operator in $L_2(n, A)$ onto the space of functions invariant under permutations of the arguments. Expanding

$$\frac{1}{V} \ln \Xi$$

in powers of ξ, we determine, as before, the coefficients $b_n(V)$.

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* For this, for example, nonnegativity of $v(x)$ is sufficient.

** The scattering operator S_Λ is closely related to the operator $1 - (E + i0 - H_n^{(0)})^{-1} V_\Lambda$. Let us perform the Fourier transform and denote by $R(E \parallel p \mid q)$ the kernel of the operator

$$\left(1 - (E + i0 - H_n^{(0)})^{-1} V_\Lambda\right)\left(1 - (E - i0 - H_n^{(0)})^{-1} V_\Lambda\right)^{-1}.$$

Then the kernel of the operator S_Λ is determined by the formula

$$S_\Lambda(p \mid q) = R(p^2 \parallel p \mid q).$$

Denote by $\tilde{b}_n^0(V)$ the coefficients obtained from $\tilde{b}_n(V)$ by replacing H_k by $H_k^{(0)}$ $(k = 1, 2, \dots)$.

Consider a decomposition of Λ into n numbers into nonintersecting subsets $\Lambda_1, \Lambda_2, \dots$. Let n_k, as before, denote the number of subsets containing k numbers. By P_{Λ_k} we shall denote the projection operator in $L_2(n, \Lambda)$ onto the subspace of functions symmetric in the variables whose indices form the set Λ_k. By P_Λ we denote the product of all P_{Λ_k}, and by T_Λ the operator equal to $(1!)^{n_1}(2!)^{n_2} \cdots P_\Lambda$.

Theorem 3. Under the same assumptions on $v(x)$ and $F(z)$ as in Theorem 1, in the Bose case there exists the limit $\tilde{b}_n = \lim_{V\to\infty} \tilde{b}_n(V)$, which is equal to

$$\tilde{b}_n = \tilde{b}_n^0 - \frac{1}{2\pi i \cdot n!} \times \tag{15}$$

$$\times \operatorname{sp}_1 \int F(z) \frac{d}{dz} \sum_\Lambda (-1)^{n_1+n_2+\cdots-1} (n_1+n_2+\cdots-1)!\, T_\Lambda \ln\left(1 - (z - H_n^{(0)})^{-1} V_\Lambda\right) dz.$$

Here the trace in this formula is understood in the same sense as in Theorem 1.*

To each monolithic complex whose vertices form the set $M = (i_1, \dots, i_n)$, associate the function

$$E_M^{(s)}(p_{i_1}, \dots, p_{i_n}) = \sigma^{(s)}(p_{i_1}, \dots, p_{i_n} \mid p_{i_1}, \dots, p_{i_n}),$$

where

$$\sigma^{(s)}(p_1, \dots, p_n \mid q_1, \dots, q_n) =$$

$$= \sum_\Lambda (-1)^{n_1+n_2+\cdots-1} (n_1 + n_2 + \cdots - 1)!\, T_\Lambda \sigma_\Lambda (p_1 \dots p_n \mid q_1 \dots q_n)$$

and σ_Λ is the function defined above.

Theorem 4. Under the same assumptions as in Theorem 2,

$$\tilde{b}_n = \tilde{b}_n^0 + \frac{1}{n!} \sum \int F^{(k)}(p_1^2 + \cdots + p_n^2) E_{M_1}^{(s)} \cdots E_{M_k}^{(s)}\, d^{3n}p. \tag{16}$$

The sum is taken over all connected complexes $M = \{M_1, \dots, M_k\}$; the order of the derivative of the function F in the term corresponding to the complex M is equal to the number of components of the complex.

In the Fermi case there hold formulas which, in writing, coincide with (15) and (16). The difference consists in the fact that the operator P_Λ, which in the Bose case is the projection operator onto the space of symmetric functions, in the Fermi case is the projection operator onto the space of antisymmetric functions. Formulas (15), (16) are in an obvious way generalized to the case of particles of arbitrary spin.

In conclusion we emphasize once more that formulas (13) and (16) are valid in the case where there is only elastic scattering. Their extension to the general case is not automatic. As for formulas (10) and (15), they are valid for scattering of any character. A typical condition under which there is only elastic scattering is $v(x) \geq 0$, $g > 0$. When the sign of g is changed, inelastic scattering arises. From formulas (10) and (15) it follows easily that b_n in both the Boltzmann and the Bose and Fermi cases is an entire function of g.** Therefore, in the case $v(x) \geq 0$, $g < 0$, the coefficients b_n can be obtained from (13) and (16) by analytic continuation in g. The coefficients b_3 were studied earlier by Pais and Uhlenbeck with the aid of perturbation theory ([4]).

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[4] Pais, Uhlenbeck, Phys. Rev., **116**, No. 2 (1959).

* In contrast to the Boltzmann case, the operator standing under the integral sign is not an operator with convergent trace even in the space $L_2^{(0)}(n)$. Therefore in formula (15) one cannot use the invariant definition of the trace.

** The analytic properties of $\tilde{b}_n$ as a function of g depend on the analytic properties of F.

Note: Figure translations are in progress. See original paper for figures.

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