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Author

Shively, John,

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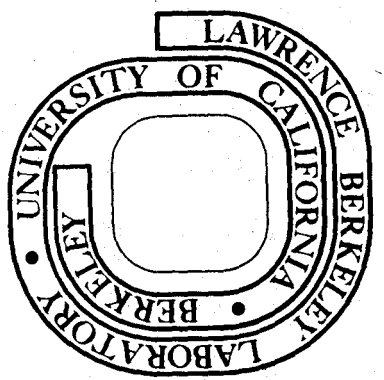
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John Shively

April 1975

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A NEW DENSITY OF STATES FORMULATION

by

John Shively

Inorganic Materials Research Division
Lawrence Berkeley Laboratory
University of California, Berkeley, California 94720

April 1975

A new formulation establishes a fundamental relationship between the spectral resolution of a Hamiltonian and the polar decomposition of its propagator which yields several expressions for the integrated density of states.

INTRODUCTION

The purpose of this paper is to establish a fundamental relationship between the spectral resolution of a Hamiltonian H and the polar decomposition of its propagator G^+ . This relationship provides a new formulation for the number $N(E)$ of eigenstates with energies less than E . As a check its derivative yields the familiar equation for the density of states $n(E)$ in terms of the trace of the propagator G^+ . The final result is similar to Lloyd's (1967) form for his integrated density of states, but the derivation here is completely different and uses exclusively the techniques of the algebra of linear operators instead of the traditional integral calculus. Specifically we use the spectral resolution theorem (Kato, 1966) and the polar decomposition theorem (Dunford and Schwartz, 1967). We begin with the former, being the more familiar of the two.

The Spectral Resolution Theorem states that any linear operator L which commutes with its conjugate L^\dagger can be expressed in the form

$$L = \sum_n \lambda_n P_n \quad (1)$$

where the λ_n are the eigenvalues of L and the P_n are its orthogonal eigenprojections

$$P_n P_m = \delta_{mn} P_n, \quad P_n^\dagger = P_n, \quad \text{and} \quad \sum_n P_n = I \quad (2)$$

The form (1) is called the spectral resolution of the linear operator L . We note that if L is hermitean, $L = L^\dagger$, then the eigenvalues λ_n are real.

The Polar Decomposition Theorem is the linear operator analogue of the polar representation for complex numbers. This theorem states

that any invertible operator L can be written in the form

$$L = R e^{iF} \quad (3)$$

where R is the unique positive operator defined by

$$R = (LL^\dagger)^{1/2} \quad (4)$$

and $U = e^{iF}$ is the unique unitary operator defined by

$$U = R^{-1}L \quad (5)$$

It is straightforward algebra to verify that $U^\dagger U = UU^\dagger = I$ so $U^\dagger = U^{-1}$ as required. Since U is unitary the phase operator F is hermitean. F can be made unique by adding or subtracting multiples of 2π from each of its eigenvalues f_n until they each lie within a prescribed interval of length 2π . By analogy with the function $\text{Arg } z$ for the phase ϕ of a complex number $z = re^{i\phi}$ we denote the phase operator F by

$$F = \text{Arg } L \quad (6)$$

If L is normal, $LL^\dagger = L^\dagger L$, then L, R, U and F all commute. If L is not invertible then the polar decomposition still exists but U is not unique.

THE FUNDAMENTAL RELATIONSHIP

The spectral resolution of the Hamiltonian H is

$$H = \sum_n E_n P_n \quad (7)$$

Its propagator $G^+(E)$ is defined as usual by

$$G^+(E) = \lim_{\epsilon \rightarrow 0} (E + i\epsilon - H)^{-1} \quad (8)$$

The polar decomposition for this propagator is

$$G^+(E) = R(E) e^{iF(E)} \quad (9)$$

where

$$R(E) = \{G^+(E)G^-(E)\}^{1/2} \quad \text{and} \quad F(E) = \text{Arg } G^+(E) \quad (10)$$

We obtain an expression for the number $N(E)$ of eigenstates of the Hamiltonian H with energy less than E simply by counting them. The number $N(E)$ of eigenstates with energy less than E is the trace of the sum of the eigenprojections on these states.

$$N(E) = \text{Tr } P(E) \quad (11)$$

where

$$P(E) = \sum_{\substack{n \\ E_n < E}} P_n \quad (12)$$

The fundamental relationship between the projection $P(E)$, arising in Eq. (12) from the spectral resolution of the Hamiltonian, and the phase operator $F(E)$, arising in Eq. (9) from the polar decomposition of the propagator, is

$$P(E) = I + \frac{1}{\pi} F(E) \quad (13)$$

This may be proven by observing from Eqs. (7), (8) and (9) that the spectral resolution of $F(E)$ must be

$$F(E) = \sum_n f_n P_n \quad (14)$$

where (a) $f_n = 0$ if $E_n < E$ because $(E+i\varepsilon-E_n)^{-1}$ is in the fourth quadrant for $\varepsilon > 0$ (b) $f_n = -\pi$ if $E_n > E$ because $(E+i\varepsilon-E_n)^{-1}$ is in the third quadrant for $\varepsilon > 0$. It may be a surprise that $f_n = -\pi$ in case (b) but that is the limit as $\varepsilon \rightarrow +0$. [We would have gotten $f_n = +\pi$ here for the phase of $G^-(E)$.] Thus Eq. (14) with (a) and (b) imply Eq. (13). Q.E.D.

The expression for $N(E)$ follows eventually from Eqs. (10), (11) and (13) as

$$N(E) = \frac{1}{\pi} \text{Tr Arg}\{-G^+(E)\} \quad (15)$$

The appearance here of the negative sign suggests that we should have used the resolvent of H instead of its propagator. Using $G^-(E)$ would change the sign, not of the propagator inside the braces, but of the whole equation.

The usual form of the density of states $n(E)$ may be obtained by differentiating Eq. (15) with respect to E . Using the formula for the derivative of the Arg function

$$\frac{d}{dz} \text{Arg } f(z) = - \frac{\text{Im } f(z)}{f^*(z)f(z)} \frac{df(z)}{dz} \quad (16)$$

we obtain the familiar result

$$n(E) = \frac{d}{dE} N(E) = - \frac{1}{\pi} \text{Im Tr } G^+(E) \quad (17)$$

We note a useful property of the function Arg

$$\text{Tr Arg } AB = \text{Tr Arg } A + \text{Tr Arg } B \quad (18)$$

even when $AB \neq BA$ and consequently when

$$\text{Arg } AB \neq \text{Arg } A + \text{Arg } B$$

By factoring $G^+(E)$ in the form

$$G^+(E) = [1-G_0^+(E)V]^{-1}G_0^+(E) \quad (19)$$

and using Eq. (18) we obtain

$$N(E) = N_0(E) - \frac{1}{\pi} \text{Tr Arg} [1 - G_0^+(E)V] \quad (20)$$

where $N_0(E)$ is the unperturbed integrated density of states. Here $H = H_0 + V$ and G_0^+ is the propagator for H_0 . By using the definition of the transition operator T

$$T = V + VG_0^+ T \quad (21)$$

we obtain the equation

$$1 + G_0^+ T = [1 - G_0^+ V]^{-1} \quad (22)$$

and hence

$$N(E) = N_0(E) + \frac{1}{\pi} \text{Tr Arg} (1 + G_0^+ T) \quad (23)$$

This is similar to Lloyd's (1967) result except he uses the reaction operator K instead of the transition operator T as in Ziman (1965).

The K matrix approach has been related by the author (Shively, 1974) to Brillouin-Wigner perturbation theory using these techniques of the algebra of linear operators and will be the subject of a forthcoming paper.

CONCLUSION

We have obtained several expressions for the number of states $N(E)$ by using the fundamental relationship between the spectral resolution of the Hamiltonian and the polar decomposition of its propagator. The usual form for the density of states followed simply by differentiation.

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REFERENCES

- Dunford, N. and J. T. Schwartz (1967), Linear Operators, Part II, Interscience, New York.
- Kato, T. (1966), Perturbation Theory for Linear Operators, Springer-Verlag, New York.
- Lloyd, P. (1967), Proc. Phys. Soc. 90, pp. 207-216.
- Shively, J. (1974), Ph.D. dissertation, Cambridge University.
- Ziman, J. M. (1965) Proc. Phys. Soc. 86, pp. 337-353.

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