C. Garwin

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RECONSTRUCTION OF THE WAVE FUNCTION FROM MATRIX ELEMENTS*

Charles Garwin

Lawrence Radiation Laboratory
University of California
Berkeley, California 94720

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ABSTRACT

We demonstrate two methods by which the wave functions of a system may be recovered from knowledge of the matrix elements of a complete set of observables.

I. INTRODUCTION

The test of any theory is its experimental confirmation, but as we all know the gap between theory and experiment is often well nigh impossible to bridge. In this paper we wish to consider some aspects of the problem of moving from experiment to theory within the context of potential theory. In particular we shall consider ourselves to be given the matrix elements of a complete set of observables, leaving aside the question of the actual experimental technique and analysis required to obtain these matrix elements, and reconstruct the wave functions of the system from this data. We shall restrict our investigation to the case of a one-dimensional system with a velocity-independent potential and no continuum states, and we shall illustrate the techniques involved by a specific application to the case of the simple harmonic oscillator.

II. THE INFINITE-ORDER DETERMINANT

Our starting point in the first technique to be illustrated are the completeness equations for the observables x and p. These equations are:

$$x\psi_n(x) = \sum_m \psi_m(x)\, x_{mn} \tag{1}$$

$$\frac{1}{i}\frac{d}{dx}\psi_n(x) = \sum_m \psi_m(x)\, p_{mn} \tag{2}$$

where the subscripts label the observed energy states of the system. Since we are given the matrix elements, ψ is the transformation function between two known representations of the irreducible set $\{x,p\}$ and hence by Schur's lemma $\psi_n(x)$ is determined by these equations up to a normalization constant.[1] The method of solution of these equations is suggested by Halpern in Ref. 1 and in this section we shall merely implement this suggestion and construct a formal solution.

The technique to be used is to solve the first set of equations for all the wave functions $\psi_m(x)$, $m \neq 0$, in terms of the ground-state wave function $\psi_0(x)$ and then substitute these results into the second equation (we need only the equation for $n = 0$), which then becomes a simple first order differential equation for $\psi_0(x)$, which can be integrated immediately. The formal solution of the first set of equations is suggested by writing out these equations for some simple case, which we take to be a harmonic oscillator potential. Then because of the vanishing of most of the matrix elements the equations assume the simple form:

$$x\psi_0(x) = \sum_m \psi_m(x)\, x_{m0} = \psi_1(x)\, x_{10}$$

$$x\psi_1(x) = \sum_m \psi_m(x)\, x_{m1} = \psi_0(x)\, x_{01} + \psi_2(x)\, x_{21} \tag{3}$$

$$x\psi_2(x) = \sum_m \psi_m(x)\, x_{m2} = \psi_1(x)\, x_{12} + \psi_3(x)\, x_{32}$$

$$\ldots \; .$$

It is then obvious that we can solve the first equation for $\psi_1(x)$ in terms of $\psi_0(x)$, the second equation for $\psi_2(x)$ in terms of $\psi_0(x)$ and $\psi_1(x)$, which we already know from the first equation, and so on. When we attempt to formalize this solution we are led to the following manipulation of equations (1), which separates out the $\psi_0(x)$ terms:

$$x\psi_n(x) = x\,\delta_{mn}\,\psi_m(x) + x\,\psi_{0n}\,\psi_0(x), \qquad m \neq 0 \tag{4}$$

$$\sum_m \psi_m(x) x_{mn} = \sum_{m\neq 0} \psi_m(x) x_{mn} + \psi_0(x) x_{0n}\,. \tag{5}$$

Combining and rearranging these equations we get:

$$\sum_{m\neq 0} (x_{mn} - \delta_{mn} x)\,\psi_m(x) = (x\,\delta_{0n} - x_{0n})\,\psi_0(x). \tag{6}$$

This is an infinite set of inhomogeneous linear equations which may be formally solved for the $\psi_m(x)$ by the usual determinental solution for linear equations, the only difference being that here the determinants are of infinite order. The use of infinite-order determinants does not pose a problem in many common potential problems since most of the

determinants will cancel, leaving us with a solution for $\psi_m(x)$ that is simply equal to a polynomial in x multiplied by $\psi_0(x)$. We shall illustrate this by solving these equations for $\psi_1(x)$ and $\psi_2(x)$ for the simple harmonic oscillator. The formal solution is (expand in minors of the first row):

$$\psi_1(x) = \frac{\begin{vmatrix} x & 0 & 0 & 0 & 0 & \cdots \\ -x_{01} & x_{21} & 0 & 0 & 0 & \cdots \\ 0 & -x & x_{32} & 0 & 0 & \cdots \\ 0 & x_{23} & -x & x_{43} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix}}{\begin{vmatrix} x_{10} & 0 & 0 & 0 & 0 & \cdots \\ -x & x_{21} & 0 & 0 & 0 & \cdots \\ x_{12} & -x & x_{32} & 0 & 0 & \cdots \\ 0 & x_{23} & -x & x_{43} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix}} \psi_0(x) = \frac{x}{x_{10}} \psi_0(x) \tag{7}$$

$$\psi_2(x) = \frac{\begin{vmatrix} x_{10} & x & 0 & 0 & 0 & \cdots \\ -x & -x_{01} & 0 & 0 & 0 & \cdots \\ x_{12} & 0 & x_{32} & 0 & 0 & \cdots \\ 0 & 0 & -x & x_{43} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix}}{\begin{vmatrix} x_{10} & 0 & 0 & 0 & 0 & \cdots \\ -x & x_{21} & 0 & 0 & 0 & \cdots \\ x_{12} & -x & x_{32} & 0 & 0 & \cdots \\ 0 & x_{23} & -x & x_{43} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix}} \psi_0(x) = \frac{x^2 - x_{10}x_{01}}{x_{10}x_{21}} \psi_0(x) \tag{8}$$

Referring to these solutions as

$$\psi_m(x) = \frac{|M_m(x)|}{|M(x)|} \psi_0(x) \tag{9}$$

we may then substitute this result into the momentum completeness equation for $\psi_0(x)$ to obtain a differential equation for $\psi_0(x)$:

$$\begin{aligned} \frac{1}{i}\frac{d}{dx}\psi_0(x) &= \sum_n \psi_n(x) p_{n0} = p_{00}\,\psi_0(x) + \sum_{m\neq 0} p_{m0}\,\psi_m(x) \\ &= p_{00}\,\psi_0(x) + \sum_{m\neq 0} p_{m0} \frac{|M_m(x)|}{|M(x)|}\psi_0(x) \\ &= \psi_0(x)\left(p_{00} + \sum_{m\neq 0} p_{m0}\frac{|M_m(x)|}{|M(x)|}\right). \end{aligned} \tag{10}$$

This equation may be immediately integrated to give:

$$\psi_0(x) = \exp\left[i \int_b^x dx \left(p_{00} + \sum_{m\neq 0} p_{m0} \frac{|M_m(x)|}{|M(x)|} \right) \right] \tag{11}$$

where the constant b is chosen to fulfill the normalization requirement. For the harmonic oscillator this equation becomes:

$$\begin{aligned} \psi_0(x) &= \exp\left[i \int_b^x dx \left(p_{10} \frac{x}{x_{10}} \right) \right] \\ &= \exp\left[i \frac{p_{10}}{x_{10}} \left(\frac{1}{2} x^2 - \frac{1}{2} b^2 \right) \right] \\ &= B \exp\left[\frac{1}{2} i \frac{p_{10}}{x_{10}} x^2 \right] \end{aligned} \tag{12}$$

which is in fact the correct solution (p_{10} is imaginary).

Of course once we have found $\psi_0(x)$ we may then go back to our solution of Eqs. (1) to generate all the $\psi_m(x)$. The potential problem is now essentially completely solved. We can use these wave functions and their observed associated energies to find the potential and the effective mass by solving the energy equations for two wave functions, say $\psi_0(x)$ and $\psi_1(x)$. These equations are:

$$\begin{aligned} V(x)\, \psi_0(x) &= E_0\, \psi_0(x) + \frac{1}{2m} \frac{d^2}{dx^2} \psi_0(x) \\ V(x)\, \psi_1(x) &= E_1\, \psi_1(x) + \frac{1}{2m} \frac{d^2}{dx^2} \psi_1(x) \end{aligned} \tag{13}$$

and the solutions are:

$$V(x) = \frac{E_0\, \psi_0(x) \frac{d^2}{dx^2} \psi_1(x) - E_1\, \psi_1(x) \frac{d^2}{dx^2} \psi_0(x)}{\psi_0(x) \frac{d^2}{dx^2} \psi_1(x) - \psi_1(x) \frac{d^2}{dx^2} \psi_0(x)} , \tag{14}$$

$$m = \frac{1}{2\left(V(x) - E_0\right)} \frac{\frac{d^2}{dx^2} \psi_0(x)}{\psi_0(x)} . \tag{15}$$

III. INTEGRATION OF CHARGE DENSITIES

Another method for finding the wave functions is also mentioned in Halpern's paper.[1] This method proceeds by using our given matrix elements to determine the matrix elements of the charge density and the charge density weighted with the momentum and then integrating the quotient of these two quantities. The relevant equations, given by Halpern, are:

$$\psi_m^*(\sigma)\,\psi_n(\sigma) = \langle E_m|\delta(x-\sigma)|E_n\rangle \tag{16}$$

$$\psi_m^*(\sigma)\,\frac{d}{d\sigma}\psi_n(\sigma) = i\langle E_m|\delta(x-\sigma)p|E_n\rangle \tag{17}$$

which may be integrated to give:

$$\psi_n(x') = \psi_n(x_0)\exp\left\{\int_{x_0}^{x'} d\sigma\,\frac{i\langle E_m|\delta(x-\sigma)p|E_n\rangle}{\langle E_m|\delta(x-\sigma)|E_n\rangle}\right\}, \tag{18}$$

m arbitrary.

The problem here is to decide upon a representation of the δ function which will make the calculation of these densities possible in practice as well as in theory. The representation that we have found is relatively easily calculable, at least for the simple case of the harmonic oscillator, is the common Fourier integral representation and we shall illustrate its use by calculating the ground state (diagonal) charge density for the harmonic oscillator. The calculation proceeds as follows (where the constant A depends on the properties of the harmonic oscillator):

$$\begin{aligned}
\psi_0^*(\sigma)\,\psi_0(\sigma) &= \langle E_0|\delta(x-\sigma)|E_0\rangle \\
&= \frac{1}{2\pi}\langle E_0|\int_{-\infty}^{\infty} d\kappa\, e^{i(x-\sigma)\kappa}|E_0\rangle \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\kappa\, e^{-i\sigma\kappa}\,\langle E_0|e^{ix\kappa}|E_0\rangle \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\kappa\, e^{-i\sigma\kappa}\sum_r \frac{1}{r'}\,x_{00}{}^r(i\kappa)^r \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\kappa\, e^{-i\sigma\kappa}\sum_{\substack{r\\ \text{even}}} \frac{1}{r'}\,\frac{(r-1)!!}{A^r}\,(i\kappa)^r \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\kappa\, e^{-i\sigma\kappa}\, e^{\left(\frac{i\kappa}{A}\right)^2/2} \\
&= \frac{A}{(2\pi)^{\frac{1}{2}}}\, e^{\frac{A^2}{2}\sigma^2}\,.
\end{aligned} \tag{19}$$

We can perform a similar calculation for Eq. (17) [using a complete set of intermediate states between $\delta(x-\sigma)$ and p], insert the results into Eq. (18) and perform the integral to obtain the wave function.

IV. SUMMARY

We have discussed two methods for reconstruction of wave functions from matrix elements. These methods provide a relatively simple formal transition between experiment and theory. Unfortunately these techniques appear to have little practical value because the various infinite series used are not amenable to approximation.

FOOTNOTES AND REFERENCES

* This work was done under the auspices of the U.S. Atomic Energy Commission.

1. M. B. Halpern, Phys. Rev. 164, 1878 (1967).

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LAWRENCE RADIATION LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720