And for $m=0$

$$\eta_{J-1}{}^{J,0}=(\tan\epsilon+\cot\epsilon)^{-1}[\cot\epsilon\eta_\alpha+\tan\epsilon\eta_\beta+(J/J+1)^{-\frac{1}{2}}(\eta_\alpha-\eta_\beta)],$$
$$\eta_{J+1}{}^{J,0}=(\tan\epsilon+\cot\epsilon)^{-1}[\tan\epsilon\eta_\alpha+\cot\epsilon\eta_\beta-(J/J+1)^{\frac{1}{2}}(\eta_\alpha-\eta_\beta)], \quad (A12)$$

where

$$\eta_L{}^{Jm}=\exp(i\delta_L{}^{Jm})\sin\delta_L{}^{Jm}, \text{ etc.}$$

Thus the phase shifts for a given J are expressed in terms of the real parameters ϵ, δ_α, δ_β.

To make use of these formulas, it is further necessary to show how the parameter and the eigen phase shifts may in practice be determined from the solutions which are obtained in the numerical solutions of the coupled tensor equations. We suppose that two independent solutions satisfying the boundary conditions have been determined, as for example by so choosing the amplitudes and slopes at the core as to satisfy the orthogonality condition.[6] These solutions are asymptotically of the form (we consider the $J=1$ even parity state)

$$\psi_i{}^m=\sin(kr+\delta_i)\mathcal{Y}_{101}{}^m+\beta_i\sin(kr-\pi+\sigma_i)\mathcal{Y}_{121}{}^m, \quad (A13)$$

where δ_i and σ_i are the (in general unequal) phase shifts for the S and D waves and β_i is a parameter determining the relative asymptotic amplitude of S and D waves. From these two solutions we construct the linear combinations

$$\psi_\rho{}^m=\psi_1{}^m+\rho\psi_2{}^m. \quad (A14)$$

If we now impose the condition that the phase shift in the S and D waves be equal, thus determining the eigen phases, we find a condition on ρ and further an expression for $\tan\delta_\rho$,

$$\frac{\sin\delta_1+\rho\sin\delta_2}{\cos\delta_1+\rho\cos\delta_2}=\frac{\beta_1\sin\sigma_1+\rho\beta_2\sin\sigma_2}{\beta_1\cos\sigma_1+\rho\beta_2\cos\sigma_2}=\tan\delta_\rho. \quad (A15)$$

This gives a quadratic equation for ρ; the two roots determine the two eigen phase shifts. Thus we can write for the solution $\psi_\alpha{}^m$:

$$\psi_\alpha{}^m=A_\alpha[\sin(kr+\delta_\alpha)\mathcal{Y}_{101}{}^m+\tan\epsilon\sin(kr+\delta_\alpha-\pi)\mathcal{Y}_{121}{}^m], \quad (A16)$$

where $\tan\epsilon$ from comparison with Eq. (A1) is, using Eq. (A15),

$$\tan\epsilon=\frac{\beta_1\sin\sigma_1+\rho_\alpha\beta_2\sin\sigma_2}{\sin\delta_1+\rho_\alpha\sin\delta_2}. \quad (A17)$$

This completes the construction from the two original solutions of the necessary parameters.

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Space-Time Representation in Wave Mechanics: Illustration of the Method

MALCOLM K. BRACHMAN
Texas Instruments Incorporated, Dallas, Texas

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The basic equations of a new space-time representation are derived in a heuristic fashion, and a simple application is presented to illustrate the point of view.

A NEW space-time representation has been developed by Hellund and the present author.[1] This paper provides a heuristic derivation of the Schrödinger equation in the new representation and illustrates its solution by considering the square-well potential.

THE SCHRÖDINGER EQUATION

We consider a one-dimensional system with a Hamiltonian $H(-i\hbar\partial/\partial x, x)$ in the Schrödinger representation. The Hamiltonian is assumed to have the form

$$H=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)=T+V. \quad (1)$$

The wave function $\Psi(x,t)$ satisfies the Schrödinger equation

$$H\Psi=i\hbar(\partial\Psi/\partial t). \quad (2)$$

Our task is to find the form of this equation in the new representation.

The one-dimensional space is split into cells by the points of division $x=L_\sigma$, $\sigma=0, \pm1, \pm2, \cdots$, with $L_0=0$. The σth cell is bounded by the abscissas L_σ and $L_{\sigma-1}$, and its length is $l_\sigma=L_\sigma-L_{\sigma-1}$. In the σth cell there is an orthonormal set of functions, $\varphi_{j\sigma}(x)$, which is defined only within the cell. These functions may be conveniently chosen to be of exponential form, and may be written

$$\varphi_{j\sigma}(x)=\frac{h(\sigma)}{\sqrt{l_\sigma}}e^{ik_{j\sigma}x},\ j=0, \pm1, \pm2, \cdots. \quad (3)$$

[1] E. J. Hellund and M. K. Brachman, Phys. Rev. 92, 822 (1953).

The k's satisfy the fundamental relationship,

$$k_{j\sigma}l_\sigma = 2\pi j, \tag{4}$$

and the function $h(\sigma)$ is defined as follows:

$$h(\sigma) = S(x - L_{\sigma-1}) - S(x - L_\sigma), \tag{5}$$

where

$$S(x) = 1, \quad x > 0, \tag{6a}$$

$$= 0, \quad x < 0. \tag{6b}$$

Thus $S(x)$ is the Heaviside unit function, and $h(\sigma)$ is seen to equal unity for $L_{\sigma-1} < x < L_\sigma$ and to vanish otherwise. We now abandon rigor and proceed, finding that it will become necessary to discard infinite terms. We note first that (5) may be differentiated to yield

$$dh(\sigma)/dx = \delta(x - L_{\sigma-1}) - \delta(x - L_\sigma), \tag{7}$$

where $\delta(x)$ is the Dirac delta function. We define

$$C_{j\sigma} = \int_{-\infty}^{\infty} \varphi_{j\sigma}^*(x)\Psi(x,t)dx, \tag{8}$$

and assume the validity of the expansion

$$\Psi(x,t) = \sum_j C_{j\sigma}\varphi_{j\sigma}. \tag{9}$$

The basic task is to project the Schrödinger equation (2) into the σth cell, or more properly, to evaluate both sides of the equation

$$(\varphi_{j\sigma}, H\Psi) = (\varphi_{j\sigma}, i\hbar\partial\Psi/\partial t), \tag{10}$$

where the customary notation for a scalar product has been employed.

The result will have the form

$$\sum_{j'\sigma'} \{(j\sigma|T|j'\sigma') + (j\sigma|V|j'\sigma')\}C_{j'\sigma'} = i\hbar\frac{\partial}{\partial t}C_{j\sigma}. \tag{11}$$

We have written

$$(j\sigma|A|j'\sigma') = \int_{-\infty}^{\infty} \varphi_{j\sigma}^* A\, \varphi_{j'\sigma'}dx, \tag{12}$$

where A is any operator. We remark that it is an obvious requirement of any consistent representation that it be isomorphic, in the sense that

$$(j\sigma|AB|j'\sigma') = \sum_{j''\sigma''} (j\sigma|A|j''\sigma'')(j''\sigma''|B|j'\sigma'), \tag{13}$$

where A and B are any appropriate operators. For convenience we introduce the notation

$$(j\sigma \,\vdots\, A \,\vdots\, j'\sigma') = (l_\sigma l_{\sigma'})^{\frac{1}{2}} \int_{-\infty}^{\infty} \varphi_{j\sigma}^* A\, \varphi_{j'\sigma'}dx. \tag{14}$$

This is patterned after the notation of Condon and Shortley,[2] but the present application will be to non-Hermitian operators.

We now proceed to calculate $(j\sigma|T|j'\sigma')$. There are two ways to do this. The first is to employ Eq. (11) with $A = (-\hbar^2/2m)(\partial^2/\partial x^2)$, and the second is to use Eq. (13) with $A = B = -i\hbar(\partial/\partial x)$. Making use of the properties of the delta function, integrating by parts, and taking account of Eq. (4) give as the result of the first method

$$(j\sigma \,\vdots\, \partial^2/\partial x^2 \,\vdots\, j'\sigma') = R + W_1, \tag{15}$$

and the second method leads to

$$(j\sigma \,\vdots\, \partial^2/\partial x^2 \,\vdots\, j'\sigma') = R + W_2. \tag{16}$$

Here R (for right) is the expression

$$R = -k_{j\sigma}^2 l_\sigma \delta_{jj'}\delta_{\sigma\sigma'} + i(k_{j'\sigma'} + k_{j\sigma}) \times [e^{i(k_{j'\sigma'} - k_{j\sigma})L_\sigma}\delta_{\sigma',\sigma+1} - e^{i(k_{j'\sigma'} - k_{j\sigma})L_{\sigma-1}}\delta_{\sigma',\sigma-1}], \tag{17}$$

and

$$W_1 = e^{i(k_{j'\sigma'} - k_{j\sigma})L_\sigma}[\delta(L_\sigma - L_{\sigma'-1}) - \delta(L_\sigma - L_{\sigma'})] - e^{i(k_{j'\sigma'} - k_{j\sigma})L_{\sigma-1}}[\delta(L_{\sigma-1} - L_{\sigma'-1}) - \delta(L_{\sigma-1} - L_{\sigma'})], \tag{18a}$$

$$W_2 = [(l_{\sigma+1})^{-1}\{\delta_{\sigma',\sigma+2}e^{i(k_{j'\sigma'}L_{\sigma+1} - k_{j\sigma}L_\sigma)} - \delta_{\sigma',\sigma}e^{i(k_{j'\sigma'} - k_{j\sigma})L}\} - (l_{\sigma-1})^{-1}\{\delta_{\sigma',\sigma}e^{i(k_{j'\sigma'} - k_{j\sigma})L_{\sigma-1}} - \delta_{\sigma',\sigma-2}e^{i(k_{j'\sigma'}L_{\sigma-2} - k_{j\sigma}L_{\sigma-1})}\}]\sum_{j''} 1. \tag{18b}$$

To obtain (16) we note that

$$(j\sigma \,\vdots\, \partial/\partial x \,\vdots\, j'\sigma') = ik_{j\sigma}l_\sigma\delta_{jj'}\delta_{\sigma\sigma'} + \delta_{\sigma',\sigma+1}e^{i(k_{j'\sigma'} - k_{j\sigma})L_\sigma} - \delta_{\sigma',\sigma-1}e^{i(k_{j'\sigma'} - k_{j\sigma})L_{\sigma-1}}, \tag{19}$$

and

$$(j\sigma \,\vdots\, \partial^2/\partial x^2 \,\vdots\, j'\sigma') = \sum_{j''\sigma''} (l_{\sigma''})^{-1} \times (j\sigma \,\vdots\, \partial/\partial x \,\vdots\, j''\sigma'')(j''\sigma'' \,\vdots\, \partial/\partial x \,\vdots\, j'\sigma'). \tag{20}$$

The expression R is, apart from a factor $-\hbar^2/2m$, that given in reference 1 for $(j\sigma|T|j'\sigma')$. The terms W_1 and W_2 arise from the nature of the mathematical processes we have used, and we discard them, remarking only that the technique discussed in reference 1 avoids these difficulties.

We now write the Schrödinger equation for our representation by combining Eqs. (9) and (17). For simplicity we limit ourselves to the case $L_\sigma = a\sigma$, *viz.*, uniform cells of length a. This restriction will be observed for the remainder of this paper, but it is, of course, unnecessary. Then Eq. (9) becomes

$$i\hbar\frac{dC_{j\sigma}}{dt} = \frac{\hbar^2}{2m}k_j^2 C_{j\sigma} + \frac{\hbar^2 i}{2ma}\sum_{j'} (k_{j'} + k_j) \times \{C_{j'\sigma-1} - C_{j'\sigma+1}\} + \sum_{j'\sigma'} (j\sigma|V|j'\sigma')C_{j'\sigma'}. \tag{21}$$

[2] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Cambridge, 1935), p. 62.

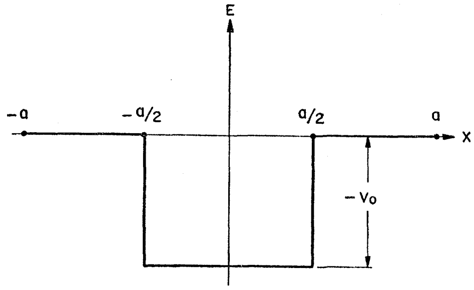

FIG. 1. The square-well potential.

Note that it is now possible to drop the subscript σ from the k's, which are the same in all cells.

An interpretation of Eq. (21) has been given in reference 1. We illustrate its use and our point of view with a simple problem and defer further development of the theory.

THE SQUARE-WELL POTENTIAL

We consider a stationary state, and write

$$C_{j\sigma}=b_{j\sigma}\exp[-(iE/\hbar)t]. \tag{22}$$

Equation (21) becomes

$$\left(\frac{\hbar^2}{2m}k_j^2-E\right)b_{j\sigma}+\frac{\hbar^2 i}{2ma}\sum_{j'}(k_{j'}+k_j)\{b_{j'\sigma-1}-b_{j'\sigma+1}\}+\sum_{j'\sigma'}(j\sigma|V|j'\sigma')b_{j'\sigma'}=0. \tag{23}$$

The problem is the familiar eigenvalue one, and requiring the determinant of the coefficients to vanish gives the secular equation for the eigenvalue of E.

For the square well of Fig. 1, the potential energy is

$$V=-V_0, \quad |x|<a/2, \tag{24a}$$

$$=0, \quad |x|>a/2. \tag{24b}$$

In accordance with our convention the σth cell extends from $(\sigma-1)a$ to σa. We have chosen the cell width equal to the width of the potential hole, but this is not a serious restriction. (On the other hand, our method requires continuity of potential at the cell boundaries.) We are interested primarily in cells 0 and 1, and a first approximation to the energy may be obtained by considering the states $j=0, \pm 1$ in both cells. We write minus one as $\bar{1}$. The requisite matrix elements obtained from Eq. (11) are diagonal in σ and take the values

$$(j0|V|j'0)=\frac{V_0}{2\pi i(j-j')}[(-1)^{j-j'}-1], \quad j'\neq j, \tag{25a}$$

$$(j0|V|j0)=-\tfrac{1}{2}V_0, \tag{25b}$$

and

$$(j1|V|j'1)=(-1)^{j'-j}(j0|V|j'0). \tag{25c}$$

For brevity we introduce

$$(\hbar^2/2ma)\epsilon=E, \tag{26}$$

and

$$(\hbar^2/2ma)v=V_0. \tag{27}$$

Inserting these into Eq. (23) yields

$$\begin{bmatrix} (2\pi)^2-\frac{1}{2}v-\epsilon & iv/\pi & 0 & 4\pi i & 2\pi i & 0 \\ -iv/\pi & -\frac{1}{2}v-\epsilon & iv/\pi & 2\pi i & 0 & -2\pi i \\ 0 & -iv/\pi & (2\pi)^2-\frac{1}{2}v-\epsilon & 0 & -2\pi i & -4\pi i \\ -4\pi i & -2\pi i & 0 & (2\pi)^2-\frac{1}{2}v-\epsilon & -iv/\pi & 0 \\ -2\pi i & 0 & 2\pi i & iv/\pi & -\frac{1}{2}v-\epsilon & -iv/\pi \\ 0 & 2\pi i & 4\pi i & 0 & iv/\pi & (2\pi)^2-\frac{1}{2}v-\epsilon \end{bmatrix}\begin{bmatrix} b_{\bar{1}0} \\ b_{00} \\ b_{10} \\ b_{\bar{1}1} \\ b_{01} \\ b_{11} \end{bmatrix}=0. \tag{28}$$

From the symmetry we find that the substitution

$$b_{j0}=b_{\bar{j}1} \tag{29}$$

reduces Eqs. (28) from six equations in six unknowns to three equations in three unknowns. Replacing $\epsilon+(v/2)$ by λ and employing (29) gives the secular equation

$$\begin{vmatrix} (2\pi)^2-\lambda & [(v/\pi)+2\pi]i & 4\pi i \\ -[(v/\pi)+2\pi]i & -\lambda & [(v/\pi)+2\pi]i \\ -4\pi i & -[(v/\pi)+2\pi]i & (2\pi)^2-\lambda \end{vmatrix}=0. \tag{30}$$

Setting $(2\pi)^2-\lambda$ equal to η and $(v/\pi)+2\pi$ equal to ω, we obtain

$$(\eta^2-16\pi^2)(\eta-4\pi^2)-2\omega^2\eta=0. \tag{31}$$

For the case $\omega\gg 1$, we find

$$\eta=\pm\sqrt{2}\omega=\pm(\sqrt{2}/\pi)v, \tag{32}$$

or

$$\epsilon=-[\tfrac{1}{2}+(\sqrt{2}/\pi)]v=-0.95v. \tag{33}$$

This corresponds to the quantum-mechanical solution,

$$E=-V_0, \tag{34}$$

which is the lowest level for the case $2ma^2V_0/\hbar^2\gg 1$.

This solution can be improved by including states of higher (absolute) j value. It is obvious that the labor involved is excessive, since the difficulty of solving the secular equation increases rapidly with its order.

Among further applications of the method that may be contemplated are the Zeeman effect, the simple harmonic oscillator, the hydrogen atom, and the Kronig-Penney model of a solid.