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One-dimensional band dispersion relations in terms of $SU(2)$ representations

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In honor of Martin Peter's 60th birthday

Abstract. The properties of the representions of the symmetry operations of the one-dimensional Schrodinger's equation are sufficient to determine, abstractly, the values for the 'allowed' ranges of energies for which the solutions of Schrodinger's equation are finite. A small set of representations which are useful factors of the representations for quite complicated translational symmetry are derived. The dispersion relationship between the wave vector and the allowed energy bands is derived. The form these dispersion equations assume is illustrated in a few special cases. It is pointed out that this approach, based on the representation for finite translations, is compatible with the computer literacy which present day students can be assumed to possess. Discussion of this type of material can provide a non-trivial excuse to use some of the powerful tools of the theory of groups.

CONTENTS

1. Salutatory Preface

It is a pleasure to be able to offer this contribution to the observance of Professor Peter's 60th birthday. I am grateful for the years we worked together as colleagues at MIT. And when he left MIT, through our continuing friendship, I have found gratification in following his career. It has been a productive career with many facets; his scientific achievements, his academic leadership, his community involvement, and his role as a caring family man. As a creative person, Professor Peter, as do all creative people, owed Society for providing him the opportunity to realize those gifts. He has repaid that debt bountifully. May he have many more decades of work now, doing just those things that are pleasing to himself!

1.1. *A bit of history*

When Professor Peter came to work with us at MIT nearly 40 years ago we were all favorably impressed by this large, gentle, intelligent Swiss student. Time was to show his influence on us all. First, his physical strength was a certain factor, when coupled with his fun loving side. He would, just to impishly challenge the lesser bodies, lift a large electro-magnet and put it in the middle of some one's desk during that person's absence. The opportunity often presented itself, for example, when he left after working late at night in the laboratory. The late Professor Richard Mattuch was half the size of Professor Peter. I remember him arriving one morning at the laboratory riding his unicycle. He then had to patiently play the role of a butt of our laughter as he struggled to clear his desk of a magnet. But the strength of the intellect of Professor Peter also influenced us more often. We had the custom of having study seminars which met once a week, with a topic which one might call 'cultural', given the daily needs of our work. Professor Peter organized a set of seminars on group theory. We were led carefully through Schur's lemma, and so on. His introduction to Schur's lemma, and to its meaning, certainly gave us the boost we needed to make the clarity and elegance of this thing of beauty – the theory of groups – useful to us in our much more mundane work. I have collected in this paper some calculations in an attempt to show some of this beauty. I am happy to dedicate this paper to Professor Peter in this Festschrift in remembrance of those associations we had nearly four decades ago.

2. Introduction

As a pedagogue I have often tried to understand the reason for the dichotomy of wave and matrix mechanics having been used so little as a tool to describe the intellectual content of quantum mechanics. It is obvious that to say that matrix mechanics concerns itself with the properties of the representations of the symmetry operations of the system, the $\mathscr{H}$ in $\mathscr{H}\psi$, and that wave mechanics concerns itself with the properties of the basis vectors, the ψ in $\mathscr{H}\psi$, glosses over the intellectual content of the dichotomy. It is like saying that the Holy Grail is a cup! It misses the historical, intellectual, and analytical content of the subject.

In the theory of rotational spectroscopy the distinction is stunning. The rotational degrees of freedom depend only upon rotation symmetry operations, i.e., the identity is the translation symmetry representation. So the system is quite simply described by the properties of the commutators of the angular momentum operators. But much early work was carried out using wave mechanics [1]. The wave-mechanics papers are long and filled with the manipulation of hypergeometric functions, and the discussion of their arcane properties. Cohorts of functions march across the pages, garlanded in superscripts, and with an underbrush of subscripts dragging at their feet. The effect of a comparison of this approach with the work of O. Klein which developed the properties of the rotational symmetry representations from the Lie algebra of the angular momentum components, is indeed stunning; the power and simplicity of the representational approach is clearly evident. But as we know the success of representational quantum mechanics as it is applied to prosaic problems has been decidedly underwhelming . . .

The situation described above requires a book for its treatment. Let me, here, give only a suggestion of what might be discussed. For an example it is appropriate to take one that includes computer literacy. Wave mechanical band theory in one dimension involves the selection of basis vectors, the wave functions, which behave 'properly' as one approaches the singularities of the potential and infinity. The most simple condition is that the wave function remain finite. When one works with basis vectors which are described as continuous functions of the coordinate and explicitly integrates Schrodinger's equation toward infinity, one can, with the use of some mathematical virtuosity, predict the behavior as the solution approaches infinity. Performing this routine on a computer is impossible. One can not 'approach infinity' since any distance described by a computation is finite. Continuing the computation simply increases the accumulated round-off error without bounds.

If, instead, one studies the representations of the translational symmetry operations for Schrodinger's equation with a computer, one need only explore representations for finite translations; the invariants of the representations for finite translations allow one to determine if the wave function they generate will behave properly as one approaches infinity. In other words, a study of matrix mechanics is more appropriate for a computation literate society. This point will become more credible if we carry out some explicit computations.

3. Translation representations for Schrodinger's equation

If we restrict ourselves to realistic potentials having denumerable discontinuities and integrable singularities, we can represent them by using a comb array of δ-functions with weight for each δ-function being given by the integral of the potential on the infinitismal interval that includes the individual δ-function. The integral of Schrodinger's equation can then be performed across a given δ-function. This procedure yields the following set of equations from which the representations for the infinitismal translation symmetry operator may be determined; (2)

$$V(x) \Rightarrow \sum \bar{V}_n \varepsilon \delta(x - n\varepsilon); \qquad \bar{V}_n = \frac{1}{\varepsilon} \int_{n\varepsilon}^{(n+1)\varepsilon} V(x)\, dx$$

$$0 = \int_{n\varepsilon-}^{n\varepsilon+} (\mathscr{H} - E)\psi(x)\, dx \Rightarrow -\psi'(n\varepsilon+) + \psi'(n\varepsilon-) + \frac{v^2}{a^2} \bar{V}_n \varepsilon \psi(n\varepsilon)$$

$$\text{unit energy} = v^2 = \frac{2ma^2}{\hbar^2}; \qquad \text{unit length} = a; \qquad \psi(n\varepsilon+) = \psi(n\varepsilon-)$$

The last equation states the need for continuity of the wave function with integrable potentials, or with particle conservation. This set of equations must be augmented by the double integral of Schrodinger's equation for free-space translation in the interval between δ-functions. In this interval the solutions to Schrodinger's equation, which allow a convenient local isomorphism of the wave function of be drawn with spinors, are the exponential phasors, $\exp(\pm ikx)$, where $k = v\sqrt{E}$. The particular solution will be some linear combination of these phasors, a similarity transformation. For completeness we must note that there is a singular solution for $k = 0$ which can not be obtained from the phasor solution by any similarity transformation. This is the solution, $\psi = Ax + B$. To include this solution in our discussion presents no difficulties. It will not be considered here explicitly, in the interest of simplifying the presentation. One can use these solutions to evaluate the slopes in the equation resulting from the first integral of Schrodinger's equation through a particular δ-function. The computation that one develops by following the wave function through the infinitismal translation in this manner rapidly degenerates into some rather opaque algebra.

3.1. *Canonical macros from SU(2) for translation*

3.1.1. *Macro for infinitesimal translational.* It is preferable at this point to make use of the fact that the wave function is a linear combination of two independent parts by using a local isomorphism of the solution with spinors. In this isomorphism the amplitudes of the linear combination of solutions that determines the wave function transform under translation like the components of a spinor. Consider the translation between δ-functions. With the exponential form chosen above, one sees that the amplitudes of the components change by an amount $\exp(\pm ik\varepsilon)$ for a translation by an amount, ε. Written as a spinor representation this would be a diagonal 2×2 matrix with those elements. Call this representation the propagation representation, P. If the amplitudes of the spinor components are called u and v, then the isomorphism is expressed explicitly as follows:

$$\psi \Rightarrow \begin{pmatrix} u \\ v \end{pmatrix}, \qquad \begin{pmatrix} u(x+\varepsilon) \\ v(x+\varepsilon) \end{pmatrix} = \begin{pmatrix} \exp(ik\varepsilon) & 0 \\ 0 & \exp(-ik\varepsilon) \end{pmatrix} \begin{pmatrix} u(x) \\ v(x) \end{pmatrix} = P(\varepsilon)\begin{pmatrix} u \\ v \end{pmatrix}$$

P would, of course, correspond to a rotation of a spinor about the z-axis. In like manner, the equation for the change in slope of the wave function due to the potential and its continuity given above can be written in terms of a spinor tunnelling representation, T. Explicitly these equations assume the following form in spinor representations.

$$\begin{aligned} \psi(n\varepsilon+) &= \psi(n\varepsilon-) \\ \psi'(n\varepsilon+) &= \psi'(n\varepsilon-) + \bar{V}_n \varepsilon \psi(n\varepsilon-) \end{aligned} \Rightarrow \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}_+$$

$$= \begin{pmatrix} 1 & 1 \\ ik + \bar{V}_n\varepsilon & -ik + \bar{V}_n\varepsilon \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}_-$$

Combining these two results, one has the representation for infinitismal translation, R, which includes both the effect of the spatial displacement and the effect of the potential, and is given by the product of the tunnelling representation, T, and the free-space propagation representation, P.(3)

$$\begin{pmatrix} u \\ v \end{pmatrix}_+ = T\begin{pmatrix} u \\ v \end{pmatrix}_-; \qquad T = \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix}^{-1} \begin{pmatrix} 1 & 1 \\ ik + \bar{V}_n\varepsilon & -ik + \bar{V}_n\varepsilon \end{pmatrix}$$

$$P\left(\frac{\varepsilon}{2}\right) = \begin{pmatrix} \exp(ik\varepsilon/2) & 0 \\ 0 & \exp(-ik\varepsilon/2) \end{pmatrix}; \qquad T = \begin{pmatrix} 1 - i\dfrac{\bar{V}_n\varepsilon}{2k} & -i\dfrac{\bar{V}_n\varepsilon}{2k} \\ i\dfrac{\bar{V}_n\varepsilon}{2k} & 1 + i\dfrac{\bar{V}_n\varepsilon}{2k} \end{pmatrix}$$

With δ-function centered:

$\mathbb{1}$ = unit matrix

$$R(\varepsilon) = P\left(\frac{\varepsilon}{2}\right) T P\left(\frac{\varepsilon}{2}\right); \qquad M(\beta) = \begin{pmatrix} \cosh\beta & -\sinh\beta \\ \sinh\beta & -\cosh\beta \end{pmatrix}$$

$$R(\varepsilon) = \mathbb{1} + i\varepsilon \cdot \sqrt{E - \bar{V}_n} M(\beta) = \exp(i\varepsilon\sqrt{E - \bar{V}_n} M(\beta)); \qquad \exp\beta = \sqrt{E - \bar{V}_n}/\sqrt{E}$$

The exponential form for the infinitismal translation follows from the fact that it is an infinitismal translation, and hence equivalent to the exponential to first order in ε, the only significant order.

3.1.2. *Macro for finite translational in a constant potential.* With a constant potential the δ-function strength is constant. Hence a translation by $N\varepsilon$ is described by N successive infinitismal translations by an amount ε. The representation for successive translations in our field of representations is the matrix product of the individual representations. Explicitly:

$$\mathcal{R} = (R(\varepsilon))^N = \exp(iN\varepsilon\sqrt{E - \bar{V}_n} M(\beta))$$

A product such as this is readily evaluated, since the Cayley–Hamilton theorem shows that it can be written as a linear function of R and the identity. (See Appendix of Ref. 3). The expansion of the exponential form is trivial since the square of the matrix involved, M, is the identity. The result is:

$$\mathcal{R} = (R(\varepsilon))^N = \cos(N\varepsilon\sqrt{E-\bar{V}_n})\mathbb{1} + i\sin(N\varepsilon\sqrt{E-\bar{V}_n})M(\beta)$$

3.1.3. *Macro for finite translation in a square wave potential.* Successive translations through constant potentials of different constant magnitude is simply the product of their individual finite translation representations. For a periodic square wave, a translation by N basis cells is the Nth power of the representation for a single basis cell. This power of the representation is readily evaluated explicitly by Sylvester's theorem, for example.

$$\begin{aligned}\mathcal{R}_1\mathcal{R}_2 &= \cos\theta_1\cos\theta_2\mathbb{1} - \sin\theta_1\sin\theta_2 M(\beta_1-\beta_2)\\ &\quad + i[\cos\theta_1\sin\theta_2 M(\beta_2) + \sin\theta_1\cos\theta_2 M(\beta_1)]\end{aligned}$$

$$\theta_1 = N_1\varepsilon_1\sqrt{E-\bar{V}_1}; \qquad \theta_2 = N_2\varepsilon_2\sqrt{E-\bar{V}_2}$$

3.1.4. *Macro for finite translational in a ramp potential.* There is probably an elegant mathematical method of evaluating the product of matrices of one linearly varying parameter, but I have not been able to discover it. So for this case we must resort to tricks. We know that the eigen functions for the ramp potential are the Airy functions. Thus the spinor amplitudes of our spinor basis vectors must be related to the Airy functions by a similarity transformation. By equating magnitude and slopes of Airy and spinor solution at one point on the potential the expansion coefficients of the linear transformation that must be used are determined. The amplitudes of the spinor components at any other point are, therefore, explicitly determined by evaluating the Airy functions at that point. This verbiage translates into equations which have the following form:

$$W(x_1) = \begin{pmatrix} f(x_1) & g(x_1) \\ f'(x_1) & g'(x_1) \end{pmatrix}; \qquad K = \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix}$$

$$W(x_2)\begin{pmatrix} A \\ B \end{pmatrix} = K\begin{pmatrix} u \\ v \end{pmatrix}$$

The determinant of W is the Wronskian of the eigen solutions, so it is constant and non-zero. The W are therefore not singular, and it can be inverted to yield the eigen function expansion amplitudes in terms of the spinor amplitudes. A second point provides a second set of equations from which the transfer matrix be evaluated as:

$$\mathcal{R} = K^{-1}W(x_2)W^{-1}(x_1)K; \qquad \begin{pmatrix} u \\ v \end{pmatrix}_{x_2} = \mathcal{R}\begin{pmatrix} u \\ v \end{pmatrix}_{x_1}$$

$$\mathcal{R} = \frac{1}{2\det W}\begin{pmatrix} (\alpha+\delta) - i\left(\beta k - \frac{\gamma}{k}\right) & (\alpha-\delta) + i\left(\beta k + \frac{\gamma}{k}\right) \\ (\alpha-\delta) - i\left(\beta k + \frac{\gamma}{k}\right) & (\alpha+\delta) + i\left(\beta k - \frac{\gamma}{k}\right) \end{pmatrix}$$

$$\alpha = f(x_2)g'(x_1) - f'(x_1)g(x_2)$$
$$\beta = f(x_1)g(x_2) - f(x_2)g(x_1)$$
$$\gamma = f'(x_2)g'(x_1) - f'(x_1)g'(x_2) \qquad \{f(x), g(x)\} = \{Ai(\pm x), Bi(\pm x)\}$$
$$\delta = f(x_1)g'(x_2) - f'(x_2)g(x_1)$$

There remains a minor detail of rescaling the space coordinate so that Schrodinger's equation assumes the form of Airy's equation,

$$\frac{d^2\psi}{dx^2} = x\psi$$

For a linear potential the relevant term in Schrodinger's equation is written in terms of an electric field strength, $\mathscr{E}$, as:

$$V - E = -\mathscr{E}\left(x + \frac{E}{\mathscr{E}}\right)$$

The change of variable is thus:

$$z = -\left(x + \frac{E}{\mathscr{E}}\right) |\mathscr{E}|^{1/3}$$

$$\frac{d^2\psi}{dz^2} = \frac{\mathscr{E}}{|\mathscr{E}|} z\psi$$

3.1.5. *Macro for translation in a symmetrical triangular potential.* The equivalent of reversing the direction of propagation is complex conjugation of the spinor amplitudes, since the amplitudes vary as $\exp(\pm ikx)$, as noted above. Reversing the direction through the potential is the inverse of the forward translation representation [2]. If the representation for translation through an ascending ramp is R1, then the representation for translation through the symmetrical descending ramp is $(\mathrm{R1}^{-1})^*$. The representation for translation through the triangular potential is therefore the product $(\mathrm{R1}^{-1})^*\mathrm{R1}$. In terms of the notation used above this is written explicitly as:

$$(\mathscr{R}_{\mathrm{sym}})_{11} = (\mathscr{R}_{\mathrm{sym}})^*_{22} = \frac{1}{(\det W)^2}\left[(\alpha\delta + \beta\gamma) + i\left(\frac{\alpha\gamma}{k} - k\delta\beta\right)\right]$$

$$(\mathscr{R}_{\mathrm{sym}})_{12} = (\mathscr{R}_{\mathrm{sym}})^*_{21} = \frac{i}{(\det W)^2}\left[\frac{\alpha\gamma}{k} + \beta\delta k\right]$$

3.1.6. *Macro for translation in a* $\operatorname{sech}^2 x$ *potential.* The $\operatorname{sech}^2 x$ potential has been an interesting curiosity and has been studied often since the original discussion of Pöschel and Teller [4]. This potential is sufficiently localized so that it can be considered to be contained within a finite segment of the x-axis. What is meant by this statement is that, at distances several times the half-width of the potential, the potential has dropped to values which differ insignificantly from its value at $\pm$ infinity. The eigen functions for this potential are the hypergeometric functions, the associated Legendre functions, or the Gegenbauer polynomials [5]. As they approach ± infinity these functions reduce to simple exponential running waves. This means that the representation for finite translation in this potential is most easily determined using these two points, namely, ± infinity. On carrying out the procedure outlined above with the Airy function, one finally obtains the following result: [5]

$$V = -s(s+1)\mu^2 \operatorname{sech}^2 \mu x; \qquad \varepsilon = \sqrt{-E}; \qquad E > 0, \qquad \varepsilon\mu = \pm ik$$

$$s - \varepsilon = n, \text{ integer} \qquad\qquad E < 0, \qquad \varepsilon\mu = k$$

$$\alpha = 2\mu\varepsilon[\sqrt{A'B}\cosh(\theta_1+\theta_2) - \sqrt{AB'}\cosh(\theta_3+\theta_4)];$$

$$A = \frac{\Gamma(1+\varepsilon)\Gamma(-\varepsilon)}{\Gamma(-s)\Gamma(1+s)}$$

$$\beta = 2[\sqrt{A'B}\sinh(\theta_1+\theta_2) + \sqrt{AB'}\sinh(\theta_3+\theta_4)];$$

$$B = \frac{\Gamma(1+\varepsilon)\Gamma(\varepsilon)}{\Gamma(\varepsilon-s)\Gamma(1+\varepsilon+s)}$$

$$\gamma = 2(\mu\varepsilon)^2[\sqrt{A'B}\sinh(\theta_1+\theta_2) - \sqrt{AB'}\sinh(\theta_3+\theta_4)];$$

$$A' = \frac{\Gamma(1-\varepsilon)\Gamma(-\varepsilon)}{\Gamma(-\varepsilon-s)\Gamma(1-\varepsilon+s)}$$

$$\delta = 2\mu\varepsilon[\sqrt{A'B}\cosh(\theta_1+\theta_2) + \sqrt{AB'}\cosh(\theta_3+\theta_4)];$$

$$B' = \frac{\Gamma(1-\varepsilon)\Gamma(\varepsilon)}{\Gamma(1+s)\Gamma(-s)}$$

$$\det W = 2\mu\varepsilon$$

$$\exp\theta_1 = \sqrt{A'/B}; \quad \theta_2 = \mu\varepsilon(x_+ - x_-); \quad \exp\theta_3 = \sqrt{A/B'}; \quad \theta_4 = \mu\varepsilon(x_+ + x_-)$$

One can also quite simply obtain the translation representation for the case of a translation from the potential extremum, $x = 0$, to x approaching plus infinity. The analysis yields the result:

$$\alpha = \mu\varepsilon[D'\exp(-\mu\varepsilon x_+) + C'\exp(\mu\varepsilon x_+)];$$

$$C = \frac{\Gamma(1+\varepsilon)\sqrt{\pi}\,2^{-\varepsilon}}{\Gamma\left(\frac{\varepsilon-s}{2}\right)\Gamma\left(1+\frac{s-\varepsilon}{2}\right)}$$

$$\beta = [-C\exp(\mu\varepsilon x_+) - D\exp(-\mu\varepsilon x_+)];$$

$$D = \frac{\Gamma(1-\varepsilon)\sqrt{\pi}\,2^{\varepsilon}}{\Gamma\left(\frac{1-\varepsilon-s}{2}\right)\Gamma\left(1+\frac{s-\varepsilon}{2}\right)}$$

$$\gamma = (\mu\varepsilon)^2[-D' \exp(-\mu\varepsilon x_+) + C' \exp(\mu\varepsilon x_+)];$$

$$C' = \frac{\Gamma(\varepsilon)\sqrt{\pi}\, 2^{-\varepsilon+1}}{\Gamma\left(\frac{1+\varepsilon+s)}{2}\right)\Gamma\left(\frac{\varepsilon-s}{2}\right)}$$

$$\delta = \mu\varepsilon[-C \exp(\mu\varepsilon x_+) + D \exp(-\mu\varepsilon x_+)];$$

$$D' = \frac{\Gamma(-\varepsilon)\sqrt{\pi}\, 2^{\varepsilon+1}}{\Gamma\left(\frac{1-\varepsilon+s}{2}\right)\Gamma\left(-\frac{\varepsilon+s}{2}\right)}$$

One can learn a good deal about special functions by attempting to demonstrate that the complex conjugate of the inverse of last result multiplied by itself is equivalent to the result obtained for the symmetric potential, the preceding equation.

4. Dispersion relations

If a similarity transformation, S, exists which will diagonalize R, then we may write:

$$S^{-1}\mathscr{R}S = \Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

Since the representation is unimodular, the product of the eigen values is 1. So we may parameterize the eigen values as:

$$\lambda_1 = \exp(+i\mu a); \qquad \lambda_2 = \exp(-i\mu a)$$

where μ is either real or imaginary, or 0, or π/a, and a is the unit of distance. Note that the invariant trace is $2\cos\mu a$. Hence if the trace of R is ± 2, then the eigen values are degenerate and equal to ± 1. In this case the diagonalizing transformation is singular, and no combination of the original basis vectors gives two eigen values. This exceptional case was mentioned above, and in this case the eigen values are ± 1, $\pm 1 + b$.

We see that the dispersion equation is determined by the trace as:

$$\cos\mu a = \tfrac{1}{2}\,\mathrm{Tr}\,\mathscr{R}$$

For the representations to be compact and the solutions bounded the trace of R must be within the interval, -2 to 2. Since R is a function of the energy, E, this equation determines the ranges of 'allowed' values of the energy.

The carrying out of the explicit solution for the allowed values of energy is, in general, a meticulous task burdened with annoying details. With the use of a computer there is no problem. One calculates the trace with successive, incremented values of the energy. Those values of energy for which the trace is within the range -2 to 2 are then used to describe the allowed states. For our present purposes, it will be sufficient to discuss some interesting aspects of the resulting dispersion relationships.

4.1. *Some properties of allowed bands*

4.1.1. *Dispersion for infinitismal translation.* The trace is readily evaluated for the representation given above. It can be written, with a simple trignometric transformation, in the following convenient form:

$$\tan \theta_n = -\bar{V}_n \varepsilon / 2k$$

$$\tfrac{1}{2} \operatorname{Tr}[R(\varepsilon)] = \frac{\cos(\theta_n + k\varepsilon)}{\cos \theta_n}$$

It should be noted that this is, possibly, a more convenient form of the dispersion relation obtained by Kronig and Penney for an array of δ-functions with finite spacing. Their use of a δ-function array was *ad hoc,* since they made no effort to relate the strength of the δ-function to a real potential. Their potential showed band gaps because the unit cell size, the spacing of the δ-functions, was assumed large. An array of constant amplitude δ-functions has a continuous energy distribution with wave vector as we will see in the next section.

4.1.2. *Dispersion for translation in a constant potential.* The trace of the representation for finite translation in a constant potential is the tautology:

$$\cos \mu N\varepsilon = \cos(N\varepsilon\sqrt{E - \bar{V}_n})$$

This means that all energies greater than the potential are allowed, and all energies less than the potential give rise to an imaginary wave vector, and so are forbidden. Integrating Schrodinger's equation gives the same result almost by inspection.

4.1.3. *Dispersion for translation in a ramp potential.* The analytical expression for the trace in this case is readily written down. The real task is one of teasing out of the equation some readily digestible information. Some special cases must be considered in order to allow the Airy functions to be expressed in terms of functions with which a wide population has had some experience. These approximations exist for values of the coordinate in the intervals, $-\infty$ to $-\frac{1}{2}$, $-\frac{1}{2}$ to $\frac{1}{2}$, and $\frac{1}{2}$ to $-\infty$. We list a typical case here:

$$E > V; \qquad z = |\mathscr{E}|^{1/3}\left(x - \frac{E}{|\mathscr{E}|}\right);$$

$$\zeta = \tfrac{2}{3} z^{3/2}; \qquad \cos \mu(x_2 - x_1) = \tfrac{1}{2} \cos(\zeta_2 - \zeta_1)\left[\sqrt[4]{\frac{z_1}{z_2}} + \sqrt[4]{\frac{z_2}{z_1}}\right]$$

4.1.4. *Dispersion for translation in a symmetrical triangular potential.* Again the trace is readily evaluated. A particular case of interest can be expressed in the following approximation: the potential, V, is a symmetrical , triangular well, descending to $-V_0$ in a distance $0.1a$, $E>0$, translate from 0 to a. [6]

$$\cos \mu a = \cos[2(\zeta_2 - \zeta_1)] \cos(0.8ak) + \sin[2(\zeta_2 - \zeta_1)] \sin(0.8ak)[|\mathscr{E}|^{1/3} + |\mathscr{E}|^{-1/3}]$$

$$z_1 = \frac{E}{|\mathscr{E}|} |\mathscr{E}|^{1/3}; \qquad z_2 = \left(0.1a - \frac{E}{|\mathscr{E}|}\right) |\mathscr{E}|^{1/3}$$

$$\zeta = \tfrac{2}{3} z^{3/2}$$

The potentials for which band gaps vanish will be given by:

$$V_0\left[\left(1 + \frac{E}{V_0}\right)^{3/2} - \left(\frac{E}{V_0}\right)^{3/2}\right]^2 = \frac{s^2\pi^2 15^2}{2^2}$$

for

$$E \ll V_0, \qquad (V_0)_s = 56,\ 25\pi^2,\ 225\pi^2, \ldots,\ 56,\ 25s^2\pi^2$$

The bound states for these potentials will be given by:

$$E_{m,s} = (V_0)_s\left[1 - \left(\frac{(2m+1)15\pi}{4(V_0)_s^{1/2}}\right)^{2/3}\right]$$

4.1.5. *Dispersion for translation in a* $\operatorname{sech}^2 x$ *potential.* This potential can be used as an approximation to the preceding potential, the symmetrical triangular potential. One well-known result for the $\operatorname{sech}^2 x$ potential is that for integer values of the amplitude parameter it is reflectionless, hence there will be no band gaps. One can use this result to determine the parameters for an equivalent triangular potential for which the band gaps will disappear. With parameters which give some congruence of this potential with the triangular potential used in the preceding section, the potentials which yield no band gaps in the continuum states are [6]:

$$V(x) = -s(s+1)\mu^2 \operatorname{sech}^2 \mu x, \qquad \mu \simeq 18$$

$$V_0 = \{0, 2, 6 \cdots\}18^2 = \{0, 66, 197 \cdots\}\pi^2$$

The bound states for these potentials are:

$$E = -\frac{\mu^2}{4}[-(1+2n) + \sqrt{1 + 4(s)(s+1)}]^2, \qquad n < s$$

$$= -\mu^2\{0, 1\}, \qquad s = 1$$

$$= -\mu^2\{0, 1, 4\}, \qquad s = 2$$

The agreement with the results of the preceding section is satisfactory.

The potential also has pedagogic interest since it is a convenient vehicle with which to discuss the factorization of the representations of the Casimir invariants of Schrodinger's equation. This process is analogous to the use of ladder operators on the special functions [7]. The latter operators allow one to express the wave functions for one potential in terms of the wave function for Schrodinger's equation with the potential amplitude parameter incremented or decremented by one unit. In this way one can deduce the general form of the translation representation for a sequence of wave functions. Analytic continuation then allows one to establish the form for any variation of the potential.

5. General remarks

The discussion given here started with the derivation of the representation for an infinitismal translation in the group of Schrodinger's equation. To discuss Schrodinger's equation one uses the quasi-Euclidean algebra $su(1, 1)$, which is homomorphic to the algebra $so(2, 1)$, among several others. This is the algebra that generates the Lorentz group that leaves a space-like vector invariant. The infinitismal representation is of the non-compact, one parameter, parabolic class. Conjugate one-parameter classes are the compact, elliptical class of rotations, and the non-compact hyperbolic class of boosts. If we had demanded total abstraction for the derivation of this matrix we could have simply assumed the form as necessary for representations of the Lorentz group. The parameter could then have been determined by exploiting the homomorphism to the Schrodinger's equation in a simple case, say, when the potential is constant.

It should be clear that the strategy of using a δ-function array to simplify the construction of the representation for translation in the Lorentz group is a convenient heurism, and not an essential structure in this problem. It imbues the problem with the reality that seems to be preferred by physicists compared to mathematical abstraction.

The issue always seems to be one of discovering the mathematical structure on which to hang the physics; or of discovering the physical problem to hang on some carefully crafted mathematical structure . . . !

6. Conclusion

There are two, at least two anyway, hard facts about physics and physicists. One is that answers to problems are usually obtained by any means that is necessary, with no regard to whether it is ugly or beautiful. The answer is paramount, the method can be forgiven. The second hard fact is that, since the time of Newton, the basic problem in physics has been that of identifying the mathematical structures upon which isomorphisms can be built with which to describe particular physical systems. One wonders if matrix mechanics would have appeared sooner if non-commuting algebra, and matrix representations had been more familiar tools of physicists. Einstein was led by Grossman to consider the properties of metric geometry and to the work of Riemann on curvature. He then saw how the equations of the general theory of relativity were to be written. Would spin have been evoked earlier if physicists had had a mathematician's understanding of the properties of even dimensional representations?

Certainly representation theory combines elegance of execution with simplicity and rigor. As pedagogues are we not short changing our students by not encouraging them in a more affirmative manner to gain facility in thinking in terms of group concepts? Band theory really has nothing to do with Mathieu functions, or other special functions. By not using representation theory more frequently are we not making our students play with a short deck of cards?

REFERENCES

[1] This is understandable since many theorists were imprinted by A. Sommerfeld, and were naturally aware of the useful properties of the special functions needed for describing wave functions. It was necessary for M. Born to point out to W. Heisenberg that the funny algebra he was using to connect transition probabilities with transition frequencies which are given by energy differences was isomorphous with matrix algebra.

[2] For a more heuristic presentation of some of this material see: M. W. P. STRANDBERG, Am. J. Phys. *54*, 321 (1986).

[3] The representations for translations determined by Schrodinger's equation belong to the Lorentz group. Hence they are always factorizable as a product of a Hermitian and a unitary matrix. In the present case the tunnelling representation, T, is a product of a unitary and a Hermitian matrix, and the propagation representation, P, is unitary. In the jargon of special relativity one sees that T is a 'boost' and a 'rotation', and P is a 'rotation'. For the explicit form of the factorization in the general case see: M. W. P. STRANDBERG, Phys. Rev. *A34*, 2458 (1986). This paper also includes a list of useful references.

[4] G. PÖSCHEL and E. TELLER, Z. Phys. *83*, 143 (1933).

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