

Algebraic solutions for Schrödinger equations with time-varying potentials and time-dependent boundary conditions

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Lie algebraic methods, which have been used widely for stationary states of quantum mechanical systems are extended here to treat time-dependent problems. Difficulties may arise at points where the potential is discontinuous or has discontinuous derivatives and from certain imposed boundary conditions. The simplicity and elegance of the usual algebraic methods can be retained for such problems by redefining the domain of the operators using techniques developed by Lighthill to introduce generalized functions.

We treat a model double-well subject to time-varying external fields as well as problems with time-dependent boundary conditions.

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As examples of this technique we treat a model double-well subject to time-varying external fields as well as problems with time-dependent boundary conditions.

Consider the usual time-dependent Schrödinger equation

$$i\frac{\partial\psi}{\partial t} = H(x, t)\psi, \quad (1)$$

where

$$H(x, t) = \sum_{j=1}^n a_j(t)L_j \quad (2)$$

and L_j are operators in some Lie algebra and in general $[L_j, H] \neq 0$. For some particular operator in L_j , L say, we may make the transformation

$$\psi = \exp(\alpha(t)L)\phi = U\phi, \quad (3)$$

where we seek to choose $\alpha(t)$ in order to simplify (1). We have

$$i\frac{\partial U\phi}{\partial t} = HU\phi, \quad (4)$$

which implies

$$U^{-1}\left(i\frac{\partial U}{\partial t}\phi + iU\frac{\partial\phi}{\partial t}\right) = (U^{-1}HU)\phi. \quad (5)$$

Since

$$\frac{\partial U}{\partial t} = \frac{d\alpha}{dt}LU \quad (6)$$

and L commutes with U we have the transformed Schrödinger equation

$$i\frac{\partial\phi}{\partial t} = \left(U^{-1}HU + i\frac{d\alpha}{dt}L\right)\phi. \quad (7)$$

We can choose U arbitrarily; usually U is chosen to eliminate L from H or to scale the variables and we will give examples of these procedures. Initially we consider choosing $\alpha(t)$ to eliminate the operator L from the equation .

To illustrate this we consider a specific Lie algebra with operators J_0, J_+, J_- satisfying the commutation relations:

$$[J_0, J_+] = J_+, \quad [J_0, J_-] = -J_-, \quad [J_+, J_-] = 2\sigma J_0 \quad (8)$$

($\sigma = 1$ for $SO(3)$ and $\sigma = -1$ for $SO(2,1)$) but in principle it is arbitrary for algebraic purposes and we choose it to be 1) and suppose that

$$H = a(t)J_- + b(t)J_0 + c(t)J_+. \quad (9)$$

Choosing $L = J_+$ we have that $U = \exp(-\alpha(t)J_+)$ and we need to calculate $U^{-1}HU$.

To do this we use the Baker–Campbell–Hausdorff expansion:

$$\exp(pA)B\exp(-pA) = B + p[A, B] + \frac{p^2}{2}[A, [A, B]] + \dots \quad (10)$$

Applying this we obtain

$$i\frac{\partial\phi}{\partial t} = \left(a(J_- + 2\alpha J_0 - \alpha^2 J_+) + b(J_0 - \alpha J_+) + cJ_+ + i\frac{d\alpha}{dt}J_+\right)\phi, \quad (11)$$

where the time-dependence has been suppressed. In the case where a, b and c are independent of t we may choose α , also independent of t , to eliminate the term in J_+ :

$$\alpha^2 a + \alpha b - c = 0. \quad (12)$$

Clearly, algebraically there is a choice for α since there are two solutions to this quadratic equation. One particular realization is

$$J_+ = \frac{1}{2}x^2, \quad J_- = -\frac{1}{2}\frac{d^2}{dx^2} \quad \text{and} \quad J_0 = \frac{1}{4}\left(x\frac{d}{dx} + \frac{d}{dx}x\right) \quad (13)$$

and with the choice $a = c = 1$ and $b = 0$ we have the standard time-independent Schrödinger equation for the harmonic oscillator. In this case the choice of α is determined since we require the solution to vanish at $x = \pm\infty$. The two possible values are in this case $\alpha = \pm 1$.

$$\psi = \exp\left(-\alpha \frac{1}{2} x^2\right) \phi, \quad (14)$$

so $\alpha = 1 > 0$ is required.

Essentially this is a boundary condition, independent of the algebra, and in cases where the coefficients are time-dependent we also need to consider the boundary conditions carefully. In order to eliminate J_+ in these cases we need to solve

$$\alpha^2 a + \alpha b - c - i \frac{da}{dt} = 0, \quad (15)$$

which is, in general a Riccati equation and we need to specify the boundary condition which will often be the value of α at $t = t_0$ and if $\alpha(t_0) = 0$ then the transformation preserves the initial wavefunction that is

$$\psi(x, t_0) = \phi(x, t_0). \quad (16)$$

There is a difficulty with these, fairly elegant, procedures in some practical examples; these are cases where the region of the variable x is confined within finite limits or the potential is different in two or more regions.

If for example we have a $\psi(a, t) = 0$ for all t and we have transformed so that as above where now $L = J_- = -\frac{1}{2} \frac{d^2}{dx^2}$ then this boundary condition becomes:

$$\psi(a, t) = \exp(-\alpha(t)J_-)\phi(x, t) |_{x=a=0}. \quad (17)$$

This of course is an awkward boundary condition and we seek to circumvent this by considering the solution of the original problem only in $x \leq b$ where $b < a$ and $a - b$ is small and in $b < x < a$ replacing H by

$$h = H + V, \quad (18)$$

where $V(a, t)$ is infinite (so $\psi(a, t) = 0$) and $V(b, t) = 0$ and all derivatives with respect to x are also zero at $x = b$. Since $a - b$ is small the essential physics will usually be equivalent to the original problem and we are only interested in the region $x < b$ and consequently the difficulty of the awkward boundary condition has been removed; the boundary conditions are formally at $x = a$ and the solution is continuous so $\phi(b, t)$ is obtained automatically.

To simplify the Hamiltonian H we may successively use $U_1 = \exp(i\alpha(t)J_+)$ and $U_2 = \exp(i\beta(t)J_-)$ to eliminate J_+ and J_- so that we have

$$H = g(t)J_0 \quad (19)$$

and since in the chosen realization $\overline{J_0}$ is a spectrum generating operator:

$$J_0 x^n = \frac{1}{4} (2n + 1) x^n, \quad (20)$$

then the exact solution may be obtained from

$$g(t) J_0 \omega = i \frac{\partial \omega}{\partial t}, \quad (21)$$

which can be solved by separation of the variables x and t . The initial wavefunction ($t = t_0$) may, most conveniently, be expanded in terms of the eigenfunctions x^n .

Another example of an awkward boundary value problem is the double well model

$$H = \begin{cases} -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} (x + a)^2 + q(t)x & -N < x < 0 \\ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} (x - a)^2 + q(t)x & 0 < x < N \end{cases} = -\frac{1}{2} \frac{d^2}{dx^2} + V(x) + q(t)x. \quad (22)$$

Here the potential $V(x)$ is continuous at the origin but has a discontinuous derivative there. The term $q(t)x$ is a model for an applied field and transformations can be used to eliminate this term and consequently to obtain the complete analytical solution. The details of this procedure have been published [1] but in addition to the transformations it is necessary to deal with the origin in a similar way to the last problem so that in $-\varepsilon < x < \varepsilon$ we redefine H to

$$H = -\frac{1}{2} \frac{d^2}{dx^2} + V(x)W(x) + q(t)x, \quad (23)$$

where $W(x)$ is a continuous function, with continuous derivatives

$$W(0) = W^{(n)}(\pm\varepsilon) = W^{(n)}(0) = 0, \quad W(x) = 1 \mid x \mid \geq \varepsilon. \quad (24)$$

Again the region $-\varepsilon < x < \varepsilon$ is assumed small and the physics is essentially the same.

There are many ways the these additional potentials ($V(x, t)$ and $W(x)$ for the two problems) can be defined, but the way we have chosen uses a function which depends on a parameter β and was used by Lighthill [2] in his derivation of generalized functions:

$$f(\beta, x) = \begin{cases} \exp(-1/(\beta^2 - x^2)) & -\beta < x < \beta \\ 0 & \text{otherwise} \end{cases}. \quad (25)$$

The function $f(\beta, x)$ is continuous and has continuous derivatives and we have that $f(\beta, \pm\beta) = 0$ and also all the derivatives of f are zero at $x = \pm\beta$.

For the first problem (where we may allow $b = \beta$ to depend on t) we take

$$V(x, t) = \begin{cases} 0 & x < b \\ \frac{f(b, x)}{a - x} & b < x < a \end{cases}. \quad (26)$$

Note that this is infinite at $x = a$ as required and smoothly zero at $x = b$.

For the second (double-well) problem we first define

$$s_{\pm}(x) = \frac{\int_0^x f\left(1, \pm \frac{2y}{\varepsilon} - 1\right) dy}{\int_0^{\pm\varepsilon} f\left(1, \pm \frac{2y}{\varepsilon} - 1\right) dy}. \quad (27)$$

Note that $s_{\pm}(0) = 0$, $s_+(\varepsilon) = s_-(-\varepsilon) = 1$ and all derivatives of $s_+(x)$ are zero at 0 and ε . Similarly all derivatives of $s_-(x)$ are zero at 0 and $-\varepsilon$. From these definitions we may construct $W(x)$:

$$W(x) = \begin{cases} 1 & x \geq \varepsilon, \\ s_+(x) & 0 \leq x \leq \varepsilon, \\ s_-(x) & -\varepsilon \leq x \leq 0, \\ 1 & x \leq -\varepsilon. \end{cases} \quad (28)$$

Examples.

In figures 1 and 2 we give an examples of the double well (with N infinite, $a = b = 2.5$) and $q(t) = t \exp(-t)$. The light curve represents the initial wavefunction and the dark curve the wavefunction at a later time. In figure 1 the initial wavefunction is the ground state of the time-independent potential at $t = 0$ (note $q(0) = 0$) and in figure 2 the initial state is a combination of the first two eigenstates chosen to localize the initial wavefunction. In both cases the wavepacket moves but in the latter case, independently of this motion the shape of the wavefunction changes.

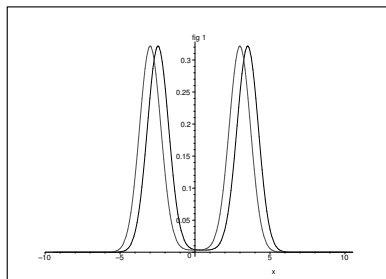


Fig. 1. Stationary initial condition

In forming stationary states we need to match the wavefunctions and their derivatives at $x = 0$ by letting $\varepsilon \rightarrow 0$ and, since N is infinite, take account of the asymptotic behaviour; this analysis is independent of the algebraic considerations. For the stationary states we have

$$H\omega = (J_+ + J_-)\omega = E\omega. \quad (29)$$

Transforming using

$$v = \exp(-\gamma J_+)\omega \quad (30)$$

leads to

$$(J_- + 2J_0)v = Ev. \quad (31)$$

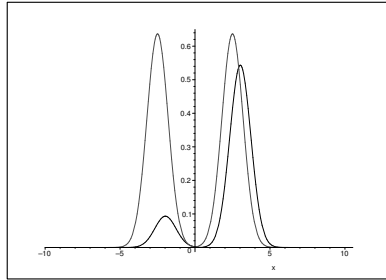


Fig. 2. Non-stationary initial condition

(Theoretically we can choose $\gamma = \pm 1$ but the choice $\gamma = i$ leads to $\omega = \exp(iJ_+)v$ and we obtain the correct asymptotic factor.)

A further transformation of the form

$$v = \exp(-\gamma_1 J_-)v_1 \quad (32)$$

can be shown to lead to a divergent expansion and we need to work with

$$(J_- + 2J_0)v = Ev \quad (33)$$

to obtain a series solution with the correct behaviour at $x = 0$ and x infinite.

Further examples

In examples such as the first problem mentioned we may have not only constraints such as

$$\psi(a, t) = 0 = \psi(-a, t) = 0, \quad (34)$$

but also the parameter a may also depend on t . The transformations may also be used, instead of eliminating an operator, to scale the problem so that the boundary conditions become time-independent.

This is achieved in the realization above using transformations of the form

$$U = \exp(-\alpha(t)J_0). \quad (35)$$

With this transformation

$$U^{-1}xU = \exp\left(\frac{\alpha}{2}\right)x \quad (36)$$

so that choosing $\exp\left(\frac{\alpha}{2}\right) = a(t)$ transforms the boundary conditions to

$$\psi(1, t) = 0 = \psi(-1, t) = 0 \quad (37)$$

independent of t . For details of the rotations in such moving boundary problems see Burrows and Cohen [3].

As an explicit example we consider

$$i\frac{\partial\psi}{\partial t} = H\psi, \quad H = -\frac{1}{2}D^2 + \frac{1}{2}\lambda x^2, \quad (38)$$

where with λ real, $\lambda > 0$ describes the standard quantal oscillator, $\lambda < 0$ a repulsive oscillator and $\lambda = 0$ a particle in a box (the range of x is restricted in each case).

We restrict the range of the space-variables to a finite closed region R , defined by

$$R : X_1 \leq x \leq X_2 \quad (39)$$

and adopt TD values for the endpoints X_1, X_2 so that

$$X_1 = -\mu L(t), \quad X_2 = \mu L(t), \quad (40)$$

where $\mu_1, \mu_2, L(t) > 0$. Just beyond these boundary points, we introduce the regions

$$R_+ : X_2 \leq x \leq X_2(1 + \varepsilon) \quad (41)$$

and

$$R_- : X_1(1 + \varepsilon) \leq x \leq X_1, \quad (42)$$

where ε is a small real positive quantity; we then impose the boundary conditions that, *for all* t

$$\psi(X_1(1 + \varepsilon), t) = \psi(X_2(1 + \varepsilon), t) = 0. \quad (43)$$

The regions R_+, R_- are intervals into which the probability density may 'leak', and formally, our model is equivalent to the modified TDSE with Hamiltonian

$$H(x, t) = -\frac{1}{2} D^2 + \frac{1}{2} \lambda x^2 + V(x, t). \quad (44)$$

Typically $L(t)$ may be oscillatory, or a pulse potential. Below we illustrate the procedure with $L(t) = 1 + \exp(-t)$ so that the moving boundary is asymptotically constant and forms a model for the process of confining the particle. A typical calculation proceeds in the following way by transforming using

$$\psi = U_1 \psi_1, \quad U_1 = \exp[i\alpha(t)J_0], \quad (45)$$

so that in R

$$i \frac{\partial \psi_1}{\partial t} = H_1 \psi_1, \quad (46)$$

with

$$H_1(x, t) = \exp(-\alpha)J_- + i\dot{\alpha}J_0 + \lambda \exp(\alpha)J_+. \quad (47)$$

Choosing $\alpha = 2 \ln(L(t))$ the boundary conditions on ψ_1 become

$$\psi_1(-\mu_1(1 + \varepsilon), t) = \psi_1(\mu_2(1 + \varepsilon), t) = 0, \quad (48)$$

while the range R becomes simply

$$-\mu_1 \leq x \leq \mu_2. \quad (49)$$

Now let

$$\psi_1 = U_2 \psi_2, \quad U_2 = \exp[-\beta(t)J_+], \quad (50)$$

Table 1.

t	$L(t)$	$P(t)$
-2	8.39	1.000
-1	3.72	1.000
0	2.00	0.995
1	1.37	0.950
2	1.14	0.891
3	1.05	0.858
4	1.02	0.855
5	1.01	0.846
6	1.00	0.838
7	1.00	0.847
8	1.00	0.845

so that we have

$$H_2(x, t) = \exp(i\alpha)J_- + (i\dot{\alpha} + 2\exp(-\alpha)\beta)J_0 + (i\dot{\beta} - i\dot{\alpha}\beta - \exp(-\alpha)\beta^2 + \lambda \exp(\alpha))J_+. \quad (51)$$

We may now choose β so that the term in J_+ is eliminated

$$i\dot{\beta} = -\lambda \exp(\alpha) + i\dot{\alpha}\beta + \exp(-\alpha)\beta^2. \quad (52)$$

In general such a Riccati equation needs to be solved numerically but here we have an analytic solution

$$\beta = k \exp(\alpha), \quad k^2 = \lambda \quad (53)$$

and from this the general solution can be obtained

$$\beta = k \exp(\alpha) \frac{B \exp(2ikt) + 1}{B \exp(2ikt) - 1}, \quad k = \sqrt{\lambda}. \quad (54)$$

We may then eliminate J_- (this may be achieved analytically by quadrature and does not involve a Riccati equation) and reach the Schrödinger equation

$$\frac{\partial \psi_3}{\partial t} = \dot{q} J_0 \psi_3, \quad \dot{q} = \dot{\alpha} - 2i \exp(\alpha)\beta, \quad (55)$$

which may be solved to give:

$$\psi_3(x, t) = U_4 \psi_3(x, t_0), \quad U_4 = \exp[q(t)J_0]. \quad (56)$$

Of course this final transformation rescales x and, to illustrate the solution it is often more convenient to use a waveform obtained earlier in the transformation. In the table below we illustrate ψ_1 with the interval R time-independent. To do this we use the measure

$$P(t) = \frac{\int_{-1}^1 |\psi_1(x, t)|^2 dx}{\int_{-1}^1 |\psi_1(x, -2)|^2 dx}. \quad (57)$$

In the table 1 we have used $L(t) = 1 + \exp(-t)$ and an initial wavefunction $\psi(x, t_0) = \exp\left(-\frac{x^2}{2}\right) \left(1 - \frac{x^2}{L(t_0)}\right)$ where so that after the first scaling transformation, $\psi_1(x, t_0)$ lies entirely in $-1 \leq x \leq 1$. From the values in the table we see that there is some leakage to the intervals R_{\pm} but asymptotically the probability of confinement is approximately 0.845 and this is fairly consistent.

References

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