

# Algebraic Method of Solution of Schrödinger's Equation of a Quantum Model

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**Abstract:** This work is aiming to show the advantage of using the Lie algebraic decomposition technique to solve for Schrödinger's wave equation for a quantum model, compared with the direct method of solution. The advantage is a two-fold: one is to derive general form of solution, and, two is relatively manageable to deal with the case of time-dependent system Hamiltonian. Specifically, we consider the model of 2-level optical atom and solve for the corresponding Schrödinger's wave equation using the Lie algebraic decomposition technique. The obtained form of solution for the wave function is used to examine computationally the atomic localization in the coordinate space. For comparison, the direct method of solution of the wave function is analysed in order to show its complication when dealing with time-dependent Hamiltonian. The possibility of using the Lie algebraic method for a qubit model (a driven quantum dot model) is briefly discussed, if Schrödinger's wave function is to be examined for the qubit localization.

**Key-Words:** Lie algebra, faithful representation, Schrödinger's wave equation, atomic localization, optical atom model.

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## 1 Introduction

In basic quantum mechanics [1], Schrödinger's wave function  $\psi(q, t)$  for a quantum model as a function of the system coordinates  $q$  at a fixed time  $t = t_0$  has the physical significance that  $|\psi(q, t_0)|^2$  is proportional to the probability of the quantum system localized at a point in the coordinate space  $q$ . For example, for an atomic model,  $|\psi(q, t_0)|^2$  is related to atomic localization in the coordinate space. Indeed, high precision position measurements are vital to physical phenomena in macroscopic systems, like Bose-Einstein condensation and laser cooling and trapping, e.g., [2]-[4]. Further, phase components of a composite wave function have their measurable effect in interference phenomena. In the present work, we examine the atomic localization related to a Hamiltonian model describing optical 2-level atom. By optical 2-level atom we mean the representation of the 2-levels by two distinct modes in an optical cavity distinguishable by their polarizations or direction of propagations. Indeed, the idea and the implementation of the new novel techniques of manipulating atom beams and atomic trajec-

tories like light present considerable interest in fundamental and applied research (see [5]-[8]). The quantum state evolution of the concerned model is investigated via Schrödinger's wave function. We use the Lie algebraic procedure of decomposition technique to solve for the Schrödinger's wave equation. A detailed study on the use of Lie algebraic methods of the type developed by Baker, Campbell, Hausdorff and Zassenhaus (BCHZ) (see ref. [9] and references therein), have been presented by Steinberg [10] and [11], to derive explicit solutions to certain class of partial differential equations. The essence of the method is the use of Lie algebraic exponential decomposition formulas of BCHZ and their matrix realization. The method was adopted to obtain general solutions of Schrödinger's wave equations for some Hamiltonian models in the field of quantum optics [12]-[16]. The advantage of the method is, its generality compared with classical methods, as we indicate in detail at the end of the paper, Sec. 6.

The algebraic technique referred to above and used in the present work may be spelled as follows (cf. [12]):

- (i) The given Schrödinger's equation generates a Lie algebra, for which we choose a basis. Hence, we seek a faithful matrix representation of low dimension for this Lie algebra (cf. [17]). For each matrix of these matrices, we find the one-parameter subgroup in order to identify the structure of the Lie group.
- (ii) The initial value problems for each element of the chosen basis, are solved separately.
- (iii) The matrix realization equation corresponding to Schrödinger's equation with respect to the faithful representation in (i) above, leads to time-dependent system of ordinary differential equations for the wave function components.
- (iv) The evolution operator of the wave equation is decomposed exponentially into product of one-parameter subgroup corresponding to the basis elements (generators), noting that each of these one-parameter subgroup satisfies the same form of a corresponding initial value problem for the basis, solved in step (ii) above. Hence, by comparison we finally get the explicit solution of Schrödinger's equation.

The paper is presented as follows. In Section 2, we introduce the Hamiltonian model with its algebra and matrix realization. The solution for the (separate) initial value problems for the basis element generators is given in Section 3 (with some detail in the Appendix A). The steps concerning the matrix realization of Schrödinger's equation and the exponential decomposition are presented in Section 4. The derived analytical expressions of the wave function are examined computationally in Section 5 regarding atomic localization for some initial state of the system (with some analytical expressions corresponding to the initial state given in Appendix B). In Section 6, we present the solution of the Schrödinger's wave equation according to the standard method. Finally, a summary and a conclusion are presented in Section 7, together with a brief reference to another quantum model, namely, pulsed driven quantum dot spin system [18], and its possible faithful matrix realization of least degree, with some detail in Appendix C.

## 2 The Model and Its Representation

The basic idea of the "optical 2-level atom" is its analogy with the system of two coupled optical radiation modes, represented as two simple harmonic oscillators, (HOs) in an optical cavity. The advantage of representing the 2-level atom by two coupled HOs is its

accurate control of the system parameters on wider ranges that are feasible for real atomic systems [5].

The Hamiltonian operator model for two-coupled modes of the electromagnetic field of unperturbed frequencies  $\omega_c \pm \omega$ , where  $\omega_c$  is the carrier frequency and for mode amplitudes that vary slowly compared with  $\omega_c$ , is of the form [5] (we take Planck constant  $\hbar = 1$ ):

$$H = \omega (a^\dagger a - b^\dagger b) + \lambda(t) (a^\dagger b + ab^\dagger) \quad (1)$$

where  $\lambda(t)$  is an arbitrary time-dependent coupling parameter and the Boson operators obey the commutation relations,

$$[a, a^\dagger] = 1 = [b, b^\dagger]. \quad (2)$$

(the symbol  $\dagger$  denotes the Hermitian conjugate).

Note that, within the context of the anti-crossing or Landau-Zener transitions phenomenon [19] and [20], the avoided crossing of the two atomic levels is governed by the frequency tuning parameter  $\omega$ , while  $\lambda(t)$  represents the opposite process of avoided crossing.

The Hamiltonian (1) may be written as combination of three operators,

$$H = \omega K_0 + \lambda(t) (K_+ + K_-) \quad (3)$$

where,

$$\begin{aligned} K_0 &= a^\dagger a - b^\dagger b, \\ K_+ &= a^\dagger b = K_-^\dagger. \end{aligned} \quad (4)$$

The Lie algebra generated by these three operators is  $\mathfrak{sl}(2)$  algebra,

$$[K_+, K_-] = K_0, \quad [K_0, K_\pm] = \pm 2K_\pm \quad (5)$$

with the *faithful* representation [21],

$$\begin{aligned} K_+ &= \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, & K_- &= \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \\ K_0 &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \end{aligned} \quad (6)$$

Note that these nontrivial traceless representation matrices preserve the physical property in which the system Hamiltonian is Hermitian (rigorous discussion regarding this point is presented in [21]-[24]).

## 3 Equations for The Generators

Schrödinger's equation for the (c-number) wave function  $\psi(q, t)$  (in the coordinate representation) for the present Hamiltonian model is

$$i \frac{\partial}{\partial t} \psi = H \psi \quad (7)$$

with arbitrary initial condition,

$$\phi(q, 0) = \psi_0(q). \quad (8)$$

For later use in the following section, we solve here the initial value problems for the three generators,  $K_0, K_{\pm}$ , namely,

$$\begin{aligned} i \frac{\partial f}{\partial t} &= K_+ f & ; f(q, 0) &= f_0(q) \\ i \frac{\partial g}{\partial t} &= K_- g & ; g(q, 0) &= g_0(q) \\ i \frac{\partial h}{\partial t} &= K_0 h & ; h(q, 0) &= h_0(q) \end{aligned} \quad (9)$$

To solve (9) we use the familiar transformation for the Boson operators (cf. [25])

$$a = \sqrt{\frac{1}{2\omega}} (\omega q_1 + i p_1) \quad ; p_1 = -i \frac{\partial}{\partial q_1} \quad (10)$$

$$b = \sqrt{\frac{1}{2\omega}} (\omega q_2 + i p_2) \quad ; p_2 = -i \frac{\partial}{\partial q_2}.$$

So, equations (9) are of the form,

$$\left(\frac{1}{2\omega}\right) \left(\omega q_1 - \frac{\partial}{\partial q_1}\right) \left(\omega q_2 + \frac{\partial}{\partial q_2}\right) f = i \frac{\partial f}{\partial t}, \quad (11)$$

$$\left(\frac{1}{2\omega}\right) \left(\omega q_2 - \frac{\partial}{\partial q_2}\right) \left(\omega q_1 + \frac{\partial}{\partial q_1}\right) g = i \frac{\partial g}{\partial t}, \quad (12)$$

$$\begin{aligned} \left(\frac{1}{2\omega}\right) [(\omega q_1 - \frac{\partial}{\partial q_1})(\omega q_1 + \frac{\partial}{\partial q_1}) \\ - (\omega q_2 - \frac{\partial}{\partial q_2})(\omega q_2 + \frac{\partial}{\partial q_2})] h = i \frac{\partial h}{\partial t}. \end{aligned} \quad (13)$$

The solutions of (11)-(13) are readily obtained (see Appendix A) in the following forms,

$$\begin{aligned} f(q_1, q_2; t) &= \sum_{n,m=-\infty}^{\infty} a_{nm} e^{\frac{i}{4}(n^2-m^2)t} \\ &\times e^{\frac{\omega}{2}(q_1^2-q_2^2)} e^{i\sqrt{\frac{\omega}{2}}[(n+m)q_1-(n-m)q_2]} \end{aligned} \quad (14)$$

$$g(q_1, q_2; t) = f(q_2, q_1; t) \quad (15)$$

$$\begin{aligned} h(q_1, q_2; t) \\ = \sum_{n,m=-\infty}^{\infty} c_{nm} e^{-i(n-m)t} e^{-\frac{\omega}{2}(q_1^2+q_2^2)} \\ \times H_n(\sqrt{\omega}q_1) H_m(\sqrt{\omega}q_2) \end{aligned} \quad (16)$$

where the coefficients  $a_{nm}$  and  $c_{nm}$  are given by

$$\begin{aligned} a_{nm} &= \frac{\omega}{4\pi^2} \int_{-\pi/\sqrt{2\omega}}^{\pi/\sqrt{2\omega}} dq'_1 \int_{-\pi/\sqrt{2\omega}}^{\pi/\sqrt{2\omega}} dq'_2 f_0(q'_1, q'_2) \\ &\times e^{\frac{\omega}{2}(q_2^2-q_1^2)} e^{i\sqrt{\frac{\omega}{2}}[(n+m)q'_1-(n-m)q'_2]} \end{aligned} \quad (17)$$

and

$$\begin{aligned} c_{nm} &= \frac{\omega}{\pi} 2^{-(n+m)} (n!m!)^{-1} \int_{-\infty}^{\infty} dq'_1 \int_{-\infty}^{\infty} dq'_2 \\ &\times h_0(q'_1, q'_2) e^{-\frac{1}{2}\omega(q_1^2+q_2^2)} H_n(\sqrt{\omega}q'_1) H_m(\sqrt{\omega}q'_2) \end{aligned} \quad (18)$$

and  $H_n(x)$  is Hermite polynomial of order  $n$ .

## 4 Matrix Realization and Exponential Decomposition

### 4.1 Matrix Realization

With the Hamiltonian form (3) and the faithful representation (6), Schrödinger's equation (7) in matrix form reads,

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= -iH\psi \\ &= -i \begin{bmatrix} \omega & \lambda(t) \\ \lambda(t) & -\omega \end{bmatrix} \psi. \end{aligned} \quad (19)$$

In components form,  $\psi = \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}$ , we have the following coupled differential equations:

$$\frac{\partial \psi_1}{\partial t} = -i\omega\psi_1 - i\lambda(t)\psi_2 \quad (20a)$$

$$\frac{\partial \psi_2}{\partial t} = i\omega\psi_2 - i\lambda(t)\psi_1, \quad (20b)$$

where the coupling parameter  $\lambda(t)$  being arbitrary function of time. The solutions of equations (20) are given in the following two cases:

#### (i) Constant Coupling.

In this case we put  $\lambda(t) = \lambda_0$  (constant) and the solutions of (20) are easily obtained in the matrix form,

$$\psi(q, t) = \begin{bmatrix} a_{11}(t) & a_{12}(t) \\ a_{21}(t) & a_{22}(t) \end{bmatrix} \psi(q, 0) \quad (21a)$$

$$\equiv A\psi(q, 0) \quad (21b)$$

where,  $a_{11}(t) = \cos(\kappa t) - \frac{i\omega}{\kappa} \sin(\kappa t)$ ,  $a_{12}(t) = a_{21}(t) = -\frac{i\lambda_0}{\kappa} \sin(\kappa t)$ ,  $a_{22}(t) = a_{11}^*(t)$  and  $\kappa = \sqrt{\lambda_0^2 + \omega^2}$ .

#### (ii) Harmonic Coupling.

In this case we take  $\lambda(t) = \lambda_0 \cos(2\nu t)$ ;  $\nu = \frac{\pi}{T}$ . The solutions of (20) can be obtained within the rotating wave approximation (RWA) in which the rapidly oscillating terms in  $e^{\pm i(\omega+\nu)t}$ , are dropped. We then get, in matrix form,

$$\psi(q, t) = \begin{bmatrix} b_{11}(t) & b_{12}(t) \\ b_{21}(t) & b_{22}(t) \end{bmatrix} \psi(q, 0) \quad (22a)$$

$$\equiv B\psi(q, 0) \quad (22b)$$

where  $b_{11}(t) = \cos(\delta t) - i\frac{\Delta}{\delta} \sin(\delta t) e^{-i\nu t}$ ,  $b_{12}(t) = -\frac{i\lambda_0}{2\delta} \sin(\delta t) e^{-i\nu t}$ ,  $b_{21}(t) = -\frac{i\lambda_0}{2\delta} \sin(\delta t) e^{i\nu t}$ ,  $b_{22}(t) = b_{11}^*(t)$ ,

$$\Delta = \omega - \nu \text{ and } \delta = \sqrt{\Delta^2 + \frac{\lambda_0^2}{4}}.$$

## 4.2 Exponential Decomposition

The formal solution of Schrödinger's equation (19) is,

$$\psi(\underline{q}, t) = e^{-iHt} \psi(\underline{q}, 0) \quad (23)$$

with  $\psi(\underline{q}, 0) = f_0(\underline{q}) g_0(\underline{q}) h_0(\underline{q})$ .

Since the Hamiltonian operator  $H$ , in (3), belongs to the Lie algebra  $\mathfrak{sl}(2)$  spanned by the three operators,  $K_{0,\pm}$ , the evolution operator  $e^{-iHt}$  is decomposed as [4],

$$e^{-iHt} = e^{-i\alpha_0(t)K_0} e^{-i\alpha_+(t)K_+} e^{-i\alpha_-(t)K_-} \quad (24)$$

where the functions  $\alpha_0(t)$  and  $\alpha_{\pm}(t)$  are to be determined.

With the matrix representation (6) one finds that the one-parameter subgroup of  $SL(2, \mathbb{R})$  associated with the generators  $K_0, K_+$  and  $K_-$  are,

$$\begin{aligned} e^{-i\alpha_0(t)K_0} &= \begin{bmatrix} e^{-i\alpha_0(t)} & 0 \\ 0 & e^{i\alpha_0(t)} \end{bmatrix}, \\ e^{-i\alpha_+(t)K_+} &= \begin{bmatrix} 1 & -i\alpha_+(t) \\ 0 & 1 \end{bmatrix}, \\ e^{-i\alpha_-(t)K_-} &= \begin{bmatrix} 1 & 0 \\ -i\alpha_-(t) & 1 \end{bmatrix}. \end{aligned} \quad (25)$$

So from (24) and (25) we get

$$e^{-iHt} = \begin{bmatrix} e_{11}(t) & e_{12}(t) \\ e_{21}(t) & e_{22}(t) \end{bmatrix} \quad (26)$$

where  $e_{11}(t) = [1 - \alpha_+(t)\alpha_-(t)] e^{-i\alpha_0(t)}$ ,  $e_{12}(t) = -i\alpha_+(t) e^{-i\alpha_0(t)}$ ,  $e_{21}(t) = -i\alpha_-(t) e^{i\alpha_0(t)}$  and  $e_{22}(t) = e^{i\alpha_0(t)}$ .

Note that the evolution operator  $e^{-iHt}$  in (23) given now by (26) is recognized as the matrix  $A$  in (21b) in the case of constant coupling or the matrix  $B$  in (22b) in the case of harmonic coupling. Thus, comparing (26) with (21b) and (22b) we get, respectively, the expressions for the three functions  $\alpha_0(t)$  and  $\alpha_{\pm}(t)$  as follows.

In the case of constant coupling:

$$\alpha_0(t) = -i \ln \left[ \cos(\kappa t) + \frac{i\omega}{\kappa} \sin(\kappa t) \right], \quad (27a)$$

$$\alpha_+(t) = \frac{\lambda_0}{\kappa} \sin(\kappa t) \left( \cos(\kappa t) + \frac{i\omega}{\kappa} \sin(\kappa t) \right), \quad (27b)$$

$$\alpha_-(t) = \frac{\lambda_0}{\kappa} \sin(\kappa t) \left( \cos(\kappa t) + \frac{i\omega}{\kappa} \sin(\kappa t) \right)^{-1}, \quad (27c)$$

and in the case of harmonic coupling,

$$\alpha_0(t) = -i \left[ i\nu t + \ln \left( \cos \delta t + i \frac{\Delta}{\delta} \sin \delta t \right) \right], \quad (28a)$$

$$\alpha_+(t) = \frac{\lambda_0}{2\delta} \sin \delta t \left( \cos \delta t + i \frac{\Delta}{\delta} \sin \delta t \right), \quad (28b)$$

$$\alpha_-(t) = \frac{\lambda_0}{2\delta} \sin \delta t \left( \cos \delta t + i \frac{\Delta}{\delta} \sin \delta t \right)^{-1}. \quad (28c)$$

## 5 Wave Function and Atomic Localization

### 5.1 Wave Function

With the decomposition formula (24) for the evolution operator  $e^{-iHt}$  one can show that [10], [12] each of the elements  $u_j = e^{-iK_j \alpha_j(t)}$  of the one-parameter subgroup corresponding with  $K_0$  and  $K_{\pm}$ , respectively, satisfies Schrödinger's type of equation,

$$i \frac{\partial}{\partial \tau_j} = K_j u_j, \quad j = \pm, 0 \quad (29)$$

where  $\tau_j = \alpha_j(t)$ .

Equation (29) have the same form of the PDEs (9). Thus, from the solutions (14)-(16), we get the action of each element  $u_j$  on the time-independent functions for  $f_0, g_0, h_0$  as follows,

$$\begin{aligned} e^{-iK_+ \alpha_+(t)} f_0(q_1, q_2) &= \sum_{r,s=-\infty}^{\infty} a_{rs} e^{\frac{i}{4}(r^2-s^2)\alpha_+(t)} e^{\frac{i\omega}{2}(q_1^2-q_2^2)} \\ &\times e^{i\sqrt{\frac{\omega}{2}}[(r+s)q_1-(r-s)q_2]}, \end{aligned} \quad (30a)$$

$$\begin{aligned} e^{-iK_- \alpha_-(t)} g_0(q_1, q_2) &= \sum_{j,k=-\infty}^{\infty} b_{jk} e^{\frac{i}{4}(j^2-k^2)\alpha_-(t)} e^{\frac{i\omega}{2}(q_2^2-q_1^2)} \\ &\times e^{i\sqrt{\frac{\omega}{2}}[(j+k)q_1-(j-k)q_2]}, \end{aligned} \quad (30b)$$

$$\begin{aligned} e^{-iK_0 \alpha_0(t)} h_0(q_1, q_2) &= \sum_{n,m=0}^{\infty} c_{nm} e^{-i(n-m)\alpha_0(t)} e^{-\frac{i\omega}{2}(q_1^2+q_2^2)} H_n, \end{aligned} \quad (30c)$$

where the normalization constants  $a_{rs}, c_{nm}$  are given in equations (17) and (18), respectively, and the constant  $b_{jk} = a_{jk} (q_1 \leftrightarrow q_2)$ .

In view of (23), (24) and (30) we have the solution of the wave function  $\psi(\underline{q}, t)$  in the form,

$$\begin{aligned} \psi(q_1, q_2; t) &= \sum_{n,m=0}^{\infty} \sum_{r,s=-\infty}^{\infty} \sum_{j,k=-\infty}^{\infty} a_{nm} b_{rs} c_{jk} e^{-i(n-m)\alpha_0(t)} \\ &\times e^{\frac{i}{4}(r^2-s^2)\alpha_+(t)} e^{\frac{i}{4}(j^2-k^2)\alpha_-(t)} \\ &\times H_n(\sqrt{\omega}q_1) H_m(\sqrt{\omega}q_2) e^{-\frac{i\omega}{2}(q_1^2+q_2^2)} \\ &\times e^{i\sqrt{\frac{\omega}{2}}\{(n+m)q_1-(n-m)q_2\} + [(r+s)q_2-(r-s)q_1]}, \end{aligned} \quad (31)$$

where the functions  $\alpha_{\pm}(t)$  and  $\alpha_0(t)$  are given by equations (27) in the case of constant coupling, or equations (28), in the case of harmonic coupling.

The solution (31) of the wave function for the Hamiltonian model (1) (or (3)) using the adopted Lie algebra approach is the principal result of this work.

### 5.2 Atomic Localization

The probability of finding the system in the coordinate space  $(q_1, q_2)$ ; i.e.,  $|\psi(q_1, q_2; t)|^2$  is conve-

niently presented in terms of the normalized variables,  $x_{1,2} = \sqrt{\omega}q_{1,2}, \tau = \omega t$  at some fixed times  $\tau = \tau_0$ . For the present illustration we consider the two HOs to be initially ( $\tau_0 = 0$ ) in their ground states,  $\psi_0(x_1, x_2) = \sqrt{\frac{\omega}{\pi}} e^{-\frac{1}{2}(x_1^2+x_2^2)}$ . (32)

Hence, the coefficients  $a_{nm}, b_{rs}, c_{jk}$  in (31) can be calculated (see Appendix B). In the case of constant coupling  $\lambda = \lambda_0; \left(\frac{\lambda_0}{\omega}\right) = O(10^{-7})$  in the optical range, the normalized probability  $|\psi(x_1, x_2)|^2 = |\psi(x_1, x_2; \tau_0)|^2 / \max(|\psi(x_1, x_2; \tau_0)|^2)$  at fixed times  $\tau = 0, \frac{\pi}{4}$  is shown in Figs. (1). The single Gaussian  $e^{-(x_1^2+x_2^2)}$  in the 3D space - Fig. 1a at  $\tau_0 = 0$  develops to many symmetric localized peaks for  $\tau_0 > 0$ , due to the oscillation induced by the interaction of the two HOs - Fig.1b (presented as log scale). Contours of the maximum localization peaks in the  $(x_1, x_2)$ -plane are shown in Fig.1c. For larger values of  $x_{1,2}, |\psi(x_1, x_2)|^2$  tends to vanish. For the other case of harmonic coupling we have very similar qualitative results in the optical range. The localization peaks of the probability  $|\psi(x_1, x_2)|^2$  along the  $x_1$ -axis (Fig. 2a) are dense, compared with that along the  $x_2$ -axis (Fig. 2b).

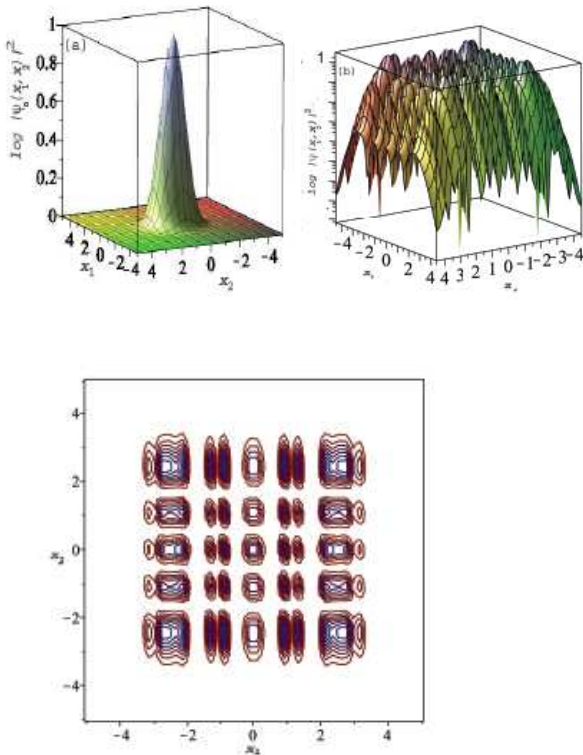


Fig.1: (a)The probability  $|\psi_0(x_1, x_2)|^2 = e^{-(x_1^2+x_2^2)}$  at  $\tau_0 = 0$   
 (b) Same as (a) but for  $|\psi(x_1, x_2)|^2$  as a log scale at  $\tau_0 = \pi/4$ .  
 (c) Contours of  $|\psi(x_1, x_2)|^2$  at  $\tau_0 = \pi/4$  in the  $(x_1, x_2)$ -plane.

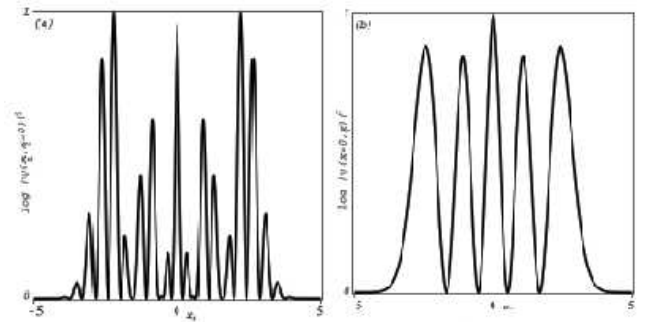


Fig.2: (a) The probability  $|\psi(x_1, x_2 = 0)|^2$  at a log scale along the  $x_1$ -axis for same data as Fig.1  
 (b) Same as (a) but for  $|\psi(x_1 = 0, x_2)|^2$  along the  $x_2$ -axis.

## 6 Standard Method of Solution

The advantage of the Lie-algebraic method of solving Schrödinger's wave equation for the present Hamiltonian model may be further justified (for comparison) if one solves the Schrödinger's equation in the standard way with arbitrary time-dependent coupling. To proceed, Schrödinger's equation (7) in the coordinate representation, with the Hamiltonian (1) and the use of the transformations (10) becomes,

$$\left[ \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_1^2} - (x_2^2 - x_1^2) + \frac{2\lambda(t)}{\omega} (x_1 x_2 - \frac{\partial^2}{\partial x_1 \partial x_2}) \right] \psi = \frac{2i}{\omega} \frac{\partial \psi}{\partial t}, \quad (33)$$

where  $x_{1,2} = \sqrt{\omega}q_{1,2}$ .

In order to solve (33) we transform  $\psi(x_1, x_2; t) \rightarrow \bar{\psi}(x, y; t)$  where,

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \cos \theta(t) & \sin \theta(t) \\ -\sin \theta(t) & \cos \theta(t) \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \quad (34)$$

one then gets (33) into the form,

$$\left[ \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial x^2} - (y^2 - x^2) + \frac{2i\dot{\theta}(t)}{\sqrt{\omega^2 + \lambda^2(t)}} (y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y}) \right] \bar{\psi} = \frac{2i}{\sqrt{\omega^2 + \lambda^2(t)}} \frac{\partial \bar{\psi}}{\partial t} \quad (35)$$

For the general case of time-dependent coupling  $\lambda(t)$ , eq. (35) (or indeed eq. (33)) is hard to deal with, even in the case of harmonic coupling parameter treated in the previous section. Here, we proceed further by assuming the integrability condition,

$$\frac{\dot{\theta}(t)}{\sqrt{\omega^2 + \lambda^2(t)}} = \beta \text{ (constant)} \quad (36a)$$

$$\text{i. e., } \theta(t) = \beta \int_0^t \sqrt{\omega^2 + \lambda^2(t')} dt' + \theta_0, \quad (36b)$$

where  $\theta_0$  is an arbitrary constant.

By letting,

$$\bar{\psi}(x, y; t) = X(x) Y(y) T(t) e^{i\beta xy} \quad (37)$$

one finds from (35),

$$\left[ \frac{1}{Y} \frac{d^2 Y}{dy^2} - (\beta^2 + 1) Y \right] - \left[ \frac{1}{X} \frac{d^2 X}{dx^2} - (\beta^2 + 1) X \right] = \frac{2i}{\Omega(t)} \frac{1}{T} \frac{dT}{dt} \quad (38)$$

where  $\Omega(t) = \sqrt{\omega^2 + \lambda^2(t)}$ .

The solution of (38) (by separation of variables), then yields the following form for  $\bar{\psi}(x, y; t)$ ,

$$\begin{aligned} \bar{\psi}(x, y; t) = & \sum_{n,m=0}^{\infty} N_{nm} e^{i\beta xy - \frac{\sqrt{\beta^2+1}(x^2+y^2)}{2}} \\ & \times H_n \left( \sqrt[4]{\beta^2+1} x \right) \\ & \times H_m \left( \sqrt[4]{\beta^2+1} y \right) e^{-i(n-m)\sqrt{\beta^2+1} \int_0^t \Omega(t') dt'} \end{aligned} \quad (39)$$

In terms of  $q_{1,2}$  we get,

$$\begin{aligned} \psi(q_1, q_2; t) = & e^{-\frac{\omega\sqrt{\beta^2+1}(q_1^2+q_2^2)}{2}} \\ & \times e^{i\beta\omega[q_1 q_2 \cos 2\theta + \frac{(q_1^2-q_2^2) \sin 2\theta}{2}]} \\ & \times \sum_{n,m=0}^{\infty} N_{nm} \\ & \times H_n \left[ \sqrt[4]{\omega^2(\beta^2+1)} (q_1 \cos \theta - q_2 \sin \theta) \right] \\ & \times H_m \left[ \sqrt[4]{\omega^2(\beta^2+1)} (q_2 \cos \theta + q_1 \sin \theta) \right] \\ & \times e^{-\frac{i(n-m)\sqrt{\beta^2+1}(\theta-\theta_0)}{\beta}}, \end{aligned} \quad (40)$$

where the normalization constants,

$$\begin{aligned} N_{nm} = & \left( \frac{\omega\sqrt{\beta^2+1}}{\pi} (m!n!)^{-1} 2^{-(m+n)} \right) \\ & \times \int_{-\infty}^{\infty} \psi(q'_1, q'_2; 0) e^{-\frac{\omega\sqrt{\beta^2+1}(q_1^2+q_2^2)}{2}} \\ & \times e^{-i\beta\omega[q'_1 q'_2 \cos 2\theta + \frac{(q_1'^2-q_2'^2) \sin 2\theta}{2}]} \\ & \times H_n \left( \sqrt[4]{\omega^2(\beta^2+1)} (q'_1 \cos \theta - q'_2 \sin \theta) \right) \\ & \times H_m \left( \sqrt[4]{\omega^2(\beta^2+1)} (q'_2 \cos \theta + q'_1 \sin \theta) \right) dq'_1 dq'_2, \end{aligned} \quad (41)$$

and  $\theta = \theta(t)$  is given by (36a).

So, within the standard method, solution of Schrödinger's wave equation is possible to derive in the case of time-dependent coupling, with imposed integrability condition, unlike the Lie algebraic approach, Sec. 4, it is solved, e.g., for harmonic coupling within the RWA.

## 7 Summary and Conclusion

We have solved Schrödinger's wave equation for the Hamiltonian model of (2-level) optical atom, (1) or (3) using the Lie-algebraic technique [9]-[12]. Provided the algebra is simple and manageable, the method has the advantage of dealing with time-dependent Hamiltonian where the matrix realization of Schrödinger's equation according to the adopted faithful representation leads naturally to time-dependent separation for the one-parameter subgroup associated with the operator generators  $K_{0,\pm}$ , eqs. (25)-(27). For the case of

time-dependent harmonic coupling we have been able to solve equations (20) within the rotating wave approximation.

Solving the wave equation using the standard approach is more tedious in the case of time-dependent coupling as compared with the presented algebraic method. Indeed, it is much convenient to deal with the coupled DEs, eqs. (20), rather than (33) when adopting any approximate or perturbative approach.

Atomic localization of the studied model is investigated computationally using the analytical solution of the wave function, for initial ground preparation of the system. Single localized Gaussian peak at initial time develops to symmetric localized peaks as time evolves. For initial states other than the ground state, lengthier analytical calculations of the coefficients in (31), (see Appendix B), with their computations, are deferred to separate presentation.

It is worth adding that, the same Lie algebraic method adopted here, based on finding a faithful matrix representations for the generators of the system Hamiltonian, can be applied to another quantum model, namely, pulsed driven quantum dot spin in the Voigt geometry [18]. The faithful matrix representation of degree 4 for the 16 generators of the system Hamiltonian are given in Appendix C. For the quantum dot localization purposes, the wave function can then be calculated similar to the procedure presented here. More non-trivial faithful matrix representations associated with generalized forms of the Lie algebra in (5) are given in [21], [22].

Further conditions of faithful matrix representation associated with deformed or non-linear Lie algebraic generalization of (5), (e.g., [26]-[29]) that correspond to some non-linear quantum optical models will be investigated in detail in a separate presentation.

In conclusion, the work in the paper emphasizes the significant advantage of using the algebraic decomposition technique for solving Schrödinger's wave equation associated with time-dependent Hamiltonian, as well provides generalized solutions compared with the direct method of solution. For higher order of matrix representation e.g., more than degree 4 or 5, depending on the system Hamiltonian, one may resort to approximate analytical approaches or computational methods to solve for the wave equation.

## Appendix A

Here we outline the derivation of the solutions of the partial differential equations (PDEs) (11)-(13).

Starting with equation (11), namely,

$$\begin{aligned} & \left( \frac{1}{2\omega} \right) \left( \omega q_1 - \frac{\partial}{\partial q_1} \right) \left( \omega q_2 + \frac{\partial}{\partial q_2} \right) f \\ & = i \frac{\partial f}{\partial t} \end{aligned} \quad (A.1)$$

and by letting  $x_1 = \sqrt{\omega} q_1$  and  $x_2 = \sqrt{\omega} q_2$ , equation (A.1) is then of the form,

$$\left[ \frac{\partial^2}{\partial x_1 \partial x_2} - x_1 x_2 + \left( x_2 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_2} \right) \right] f = -2i \frac{\partial f}{\partial t}. \quad (\text{A.2})$$

If we put

$$f = \bar{f} e^{1/2(x_1^2 - x_2^2)}, \quad (\text{A.3})$$

then we have,

$$\frac{\partial^2 \bar{f}}{\partial x_1 \partial x_2} = -2i \frac{\partial \bar{f}}{\partial t}. \quad (\text{A.4})$$

Next, we let

$$x_1 = \frac{\xi + \eta}{\sqrt{2}}, \text{ and } x_2 = \frac{\eta - \xi}{\sqrt{2}}, \quad (\text{A.5})$$

then (A.4) gives

$$\frac{\partial^2 \bar{f}}{\partial \eta^2} - \frac{\partial^2 \bar{f}}{\partial \xi^2} = -4i \frac{\partial \bar{f}}{\partial t}. \quad (\text{A.6})$$

Equation (A.6) is easily solved by the separation of variables to give finally the solution (14) for  $f(q_1, q_2; t)$ . The PDE for  $g$ , equation (12), is treated similarly. As for equation (13), this simply reduces to the form

$$\frac{1}{2\omega} \left[ \omega^2 q_1^2 - \frac{\partial^2}{\partial q_1^2} - \left( \omega^2 q_2^2 - \frac{\partial^2}{\partial q_2^2} \right) \right] h = i \frac{\partial h}{\partial t}, \quad (\text{A.7})$$

which is solved by the separation of variables in terms of the familiar Hermite polynomials, in (16).

### Appendix B

Here we present the analytical expressions for the coefficients  $a_{nm}, b_{rs}, c_{jk}$  given by (17), (18), appearing in the solution of the wave function  $\psi(q_1, q_2; t)$  in (31).

Introducing the normalized variables,

$$x_{1,2} = \sqrt{\omega} q_{1,2}, \tau = \omega t, \quad (31) \text{ takes the form,}$$

$$\begin{aligned} \psi(x_1, x_2; \tau) &= e^{-\frac{1}{2}(x_1^2 + x_2^2)} \\ &\times \sum_{n,m=0}^{\infty} a_{nm} e^{-i(n-m)\alpha_0(\tau)} e^{\frac{i(n+m)x_1}{\sqrt{2}}} \\ &\times e^{-\frac{i(n-m)x_2}{\sqrt{2}}} \frac{H_n(x_1) H_m(x_2)}{\sqrt{2}} \\ &\times \sum_{r,s=-\infty}^{\infty} b_{rs} e^{\frac{i(r^2 - s^2)\alpha_+(\tau)}{4}} e^{\frac{i(r+s)x_2}{\sqrt{2}}} e^{-\frac{i(r-s)x_1}{\sqrt{2}}} \\ &\times \sum_{j,k=-\infty}^{\infty} c_{jk} e^{\frac{i(j^2 - k^2)\alpha_-(\tau)}{4}}, \end{aligned} \quad (\text{B.1})$$

where,  $\alpha_{0,\pm}(\tau)$  in the case of constant coupling, eq. (27) have the forms,

$$\alpha_0(\tau) = -i \ln(\cos \tau + i\beta_1 \sin \tau) \quad (\text{B.2a})$$

$$\alpha_+(\tau) = \beta_2 \sin \tau (\cos \tau + i\beta_1 \sin \tau) \quad (\text{B.2b})$$

$$\alpha_-(\tau) = \beta_2 \sin \tau (\cos \tau + i\beta_1 \sin \tau)^{-1} \quad (\text{B.2c})$$

$$\text{with } \beta_1 = \sqrt{1 + \left( \frac{\lambda_0}{\omega} \right)^2} \text{ and } \beta_2 = \frac{1}{\sqrt{1 + \left( \frac{\omega}{\lambda_0} \right)^2}}.$$

To calculate the constants  $a_{nm}, b_{rs}, c_{jk}$  in (17), (18) we consider the two HOs are in their ground state,

$$\begin{aligned} \psi_0(x_1, x_2; 0) &= Q(x_1, x_2) \\ &\equiv f_0(x_1, x_2) g_0(x_1, x_2) h_0(x_1, x_2) \end{aligned} \quad (\text{B.3})$$

$$\text{where, } Q(x_1, x_2) = \sqrt{\frac{\omega}{\pi}} e^{-\frac{x_1^2 + x_2^2}{2}}.$$

From (B.3), we may choose

$$f_0(x_1, x_2) = Q(x_1, x_2), \quad (\text{B.4a})$$

$$g_0(x_1, x_2) = h_0(x_1, x_2) = 1. \quad (\text{B.4b})$$

Other choices, such as,

$$f_0(x_1, x_2) = h_0(x_1, x_2) = 1, g(x_1, x_2) = Q(x_1, x_2),$$

$$f_0(x_1, x_2) = g_0(x_1, x_2) = 1, h(x_1, x_2) = Q(x_1, x_2),$$

$$\text{or, } f_0(x_1, x_2) = g_0(x_1, x_2) = h_0(x_1, x_2) = \sqrt[3]{Q(x_1, x_2)},$$

give essentially the same qualitative results for the probability  $|\psi(x_1, x_2; \tau)|^2$ . So, specifically, for the choice (B.4) and from (17), (18) we get the following expressions,

$$\begin{aligned} a_{nm} &= \frac{1}{\pi^{3/2} \sqrt{2}} \left( \frac{\omega}{\pi} \right)^{1/4} e^{\frac{(n+m)^2}{8}} \\ &\times (\text{erf}(q_+) - \text{erf}(q_-)) \\ &\times \begin{cases} \pi & (n = m) \\ \frac{\sin[\pi(n-m)]}{n-m} & (n \neq m) \end{cases}, \end{aligned} \quad (\text{B.5a})$$

$$b_{rs} = \frac{2i}{\pi^3} e^{-rs} (\text{erf}(p_+) - \text{erf}(p_-)) \times (\text{erf}(z_+) - \text{erf}(z_-)), \quad (\text{B.5b})$$

$$c_{j,k} = \frac{\pi}{j! k!} (2)^{-2(j+k)}, \quad (\text{B.5c})$$

where,

$$q_{\pm} = \frac{1}{\sqrt{2}} \left( \pm \pi - \frac{n+m}{2} i \right),$$

$$p_{\pm} = \frac{1}{2} \left( \mp \pi i - \frac{r-s}{2} \right),$$

$$z_{\pm} = \frac{1}{2} \left( \pm \pi - \frac{r+s}{2} i \right),$$

and

$$\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-z_1^2} dz_1 \text{ is the error function of}$$

complex argument ( $z$ ),

and have used [30],

$$\int_0^{\infty} e^{-\frac{x^2}{2}} H_{2n}(x) dx = \sqrt{\frac{\pi}{2}} \frac{(2n)!}{n!}.$$

### Appendix C

Here, we refer to another basic quantum model [18] and show that it has a faithful matrix representation for the generators of its Hamiltonian model. The concerned model in [18] considers a quantum dot electron spin states in the Voigt geometry that can act as a qubit manipulated by optical pulses to achieve possible quantum gates. The model Hamiltonian describing the coupling of the quantum dot system of 4-level structure with two time-dependent optical fields can be put in the following form in the electric dipole and rotating wave approximations, [18].

$$\begin{aligned} H &= \sum_{i=1}^4 \hbar \omega_i R_i \\ &- h[\Omega_a(t) e^{-i\omega_a t} (R_{41} + R_{32}) \\ &+ \Omega_b(t) e^{-i\omega_b t} (R_{31} + R_{42}) + h.c.] \end{aligned} \quad (\text{C.1})$$

The notations are:  $\hbar \omega_i$  is the energy of the state  $|i\rangle$ ,  $\Omega_{a,b}(t)$  are the real time-dependent Rabi frequencies of the two applied fields, with frequencies  $\omega_a, \omega_b$ , respectively. The operators  $R_i = |i\rangle \langle i|$  such that  $\sum_{i=1}^4 R_i = I, R_{ji} = |j\rangle \langle i| = R_{ij}^\dagger; i, j = 1 - 4$ , from

a closed Lie algebra, satisfying the following commutation relations,

$$\begin{aligned}
 [R_i, R_j] &= 0 && ; \text{ for all } i, j = 1 - 4, \\
 [R_{ij}, R_{ji}] &= R_i - R_j && ; i \neq j, i, j = 1 - 4 \\
 [R_i, R_{ij}] &= R_{ij} && ; i \neq j \\
 [R_i, R_{ji}] &= -R_{ji} && ; i \neq j \\
 [R_i, R_{jk}] &= 0 && ; i \neq j \neq k \\
 [R_{ij}, R_{ki}] &= -R_{kj} && ; j \neq k \\
 [R_{ij}, R_{ik}] &= 0 && ; i \neq j \neq k
 \end{aligned} \tag{C.2}$$

These commutation relations in (C.2) can be summarized in the following lemma.

**Lemma 1** Let  $R_i = R_{ii}$  for  $i = 1 - 4$ . The operators  $R_{ij}$  satisfy  $R_{ij}R_{kl} = \delta_{jk}R_{il}$  and hence,  $[R_{ij}, R_{kl}] = \delta_{jk}R_{il} - \delta_{li}R_{kj}$ , for  $i, j = 1 - 4$ .

Further, we mention that, the  $n \times n$  matrices  $E_{ij}$ , of the standard basis of the vector space  $M_n(\mathbb{R})$  are called the  $n \times n$  matrix units. The entries of each  $E_{ij}$  are all zeros and 1 in its  $(i, j)$ -entry [31].

**Lemma 2** The  $n \times n$  matrix units  $E_{ij}$  satisfy  $E_{ij}E_{kl} = \delta_{jk}E_{il}$  and hence,  $[E_{ij}, E_{kl}] = \delta_{jk}E_{il} - \delta_{li}E_{kj}$ , for  $i, j = 1 - 4$ .

From the above lemmas, for  $n = 4$ , the matrix unit  $E_{ij}$  is a representation matrix for the operator  $R_{ij}$  for  $i, j = 1 - 4$ , respectively, because it satisfy (C.2). This matrix representation is faithful since, the  $E_{ij}$  are linearly independent. Also, this representation is the least degree because, the dimension of the Lie algebra is 16.

So, the present algebraic method to solve for the wave function of the model and hence the quantum dot localization can then be investigated.

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