Gauge invariance and wave packet simulations
in the presence of dipole fields

Thierry Martin*
CNLS, Theory Division, Los Alamos National Laboratory, Los Alamos, NM 87545

A method for performing wave packet simulations in dipole fields is presented. Starting from a Hamiltonian with non commuting terms, a gauge transformation leads to a new Hamiltonian which allows to calculate explicitly the evolution operator. In this new gauge, the dipole field is fully included in the vector potential. The method of Goldberg, Schwartz and Schey based on the Caley form of the evolution operator is then generalized, and the resulting scheme is applied to describe a switching device. The device is composed of a well region separated from a free region by a potential barrier, such that one bound state and one quasi level are present. For a particle initially in the ground state, transitions to the quasi level are induced by applying a dipole field, and the wave function can subsequently tunnel in the free region. The probability to tunnel in the free region exhibits a plateau structure as the wave function is emitted by “bursts” after each Rabi oscillation has been completed.

The pioneering work of Goldberg, Schey and Schwartz on numerical simulations of wave packet evolution through potential barriers and wells continues to have a deep impact on the teaching community. However, when this work first appeared, the technological means to observe and characterize experimentally such phenomenon were absent. One dimensional quantum mechanics was then considered on a rather academic level. With the recent advances in the fabrication of semiconductor nanostructures, one now has the means to design such structures using molecular beam epitaxy techniques, etc... The motivation for research in this field now comes from the hope that quantum devices may one day be used as elementary building blocks for the next generation of computers. In the following, I will describe a method which allows to simulate the evolution of a wave packet in a potential landscape, in the presence of a dipole potential. The method will be applied to describe a switching device consisting of a well, separated by a free region by a potential landscape, in the presence of a dipole potential. The method will be applied to describe a switch-
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required, such as in the case where a (small) barrier or 
well region which specify the characteristic energies of 
the problem, is coupled to a (large) continuum region, 
the expectation value $<x>$ of the position operator 
may take large values. This puts further restrictions on 
the magnitude of the time step for the simulation.

Nevertheless, a more elegant method, which exploits 
the gauge invariance property of the Hamiltonian, does 
not suffer from the same constraints. The Hamiltonian 
of Eqs. (1) and (2) is written in a gauge where the vector 
potential $A = 0$ and the scalar potential is $\phi(x, t)$. An 
alternative choice of gauge can be obtained as:

$$A' = A - \frac{\partial}{\partial x} \chi$$

$$\phi' = \phi + \frac{1}{c} \frac{\partial}{\partial t} \chi$$

(6)

(7)

Now, I choose the “new” gauge so that the scalar potential 
$\phi' = 0$. This then yields:

$$\chi(x, t) = -\frac{e \chi}{\omega} \sin(\omega t)$$

$$A'(x, t) = \frac{e \chi}{\omega} \sin(\omega t)$$

(8)

(9)

In this new gauge, the Hamiltonian is written as:

$$H' = \frac{1}{2m} \left( \frac{\hbar}{i} \frac{\partial}{\partial x} - \frac{e}{c} A' \right)^2 + V(x)$$

$$= \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + i \frac{e \hbar}{mc} A' \frac{\partial}{\partial x} + V(x) + \frac{e^2}{2mc^2} A'^2$$

(10)

The second line follows from the fact that $A'$ commutes 
with the momentum operator. In the new gauge, the 
wave function $\psi'(x, t)$ is related to the old one:

$$\psi'(x, t) = \psi(x, t) e^{-i\chi(x,t) / \hbar c}$$

(11)

Note that the Hamiltonian $H'$ does not suffer from the 
same setbacks as $H$: in each constant region of $V(x)$ all 
terms in the Hamiltonian $H'$ commute with each other, 
and consequently, the time ordering factor in the expression 
for the evolution operator $U'(t, t_0)$ can be dropped out:

$$U'(t, t_0) = \exp \left[ \frac{i}{\hbar} \int_{t_0}^{t} dt' H'(t') \right]$$

$$= \exp \left[ -i \frac{t-t_0}{\hbar} H_0 - \frac{g(t, t_0)}{m} \frac{\partial}{\partial x} - i\theta(t, t_0) \right]$$

(12)

with

$$g(t, t_0) = \frac{e}{\omega^2} (\cos(\omega t) - \cos(\omega t_0))$$

$$\theta(t, t_0) = \frac{e^2}{2\hbar mc^2} \int_{t_0}^{t} dt' A'^2(t')$$

(13)

(14)

Note that the last term in the exponential contributes 
only a time dependent phase factor to the evolution. 
Therefore, $\theta(t, t_0)$ will be omitted in the following.

I now generalize the numerical scheme of GGS to the 
problem where a vector potential is present. The elementary 
time step evolution for the wave function $\psi'$ is taken in 
the so-called Caley form:

$$\psi'(t + \delta t) = \frac{1 - \frac{i}{\hbar} \delta t H'}{1 + \frac{i}{\hbar} \delta t H'} \psi'(t)$$

(15)

or, alternatively, in the “old” gauge:

$$\psi(t + \delta t) = e^{i\chi(t+\delta t)/\hbar c} \frac{1 - \frac{i}{\hbar} \delta t H'}{1 + \frac{i}{\hbar} \delta t H'} e^{-i\chi(t)/\hbar c} \psi(t)$$

(16)

which has the advantage of being exact to order $(\delta t)^2$ 
and unitary. Taking the convention $\hbar = 1, m = 1/2, and$ 
choosing the discretized variables $x = j \delta x \ (j = 0,1,...J) , 
\ t = n \delta t \ (n = 1,2,...), \ (\psi(x, t) \equiv \psi^0_j), \ (g(t) \equiv \delta t g_n), 
\ (V(x) = V_j)$, this is rewritten as:

$$\psi_{j+1}^{n+1} (1 + i \frac{\delta t}{2} V_j) + i \lambda^{-1} (-\psi_{j+1}^n + 2 \psi_j^{n+1} - \psi_{j-1}^n)$$

$$+ i \frac{\delta t}{2 \delta x} (-i \delta \phi_j) (\psi_{j+1}^n - \psi_{j-1}^n) - i \frac{\delta t}{2 \delta x} (\psi_{j+1}^n - \psi_{j-1}^n)$$

(17)

where $\lambda = 2 \delta x^2 / \delta t$. Introducing the quantity:

$\Omega^n_j = \psi_{j+1}^n (-1 - i \delta x g_n) + \psi_j^n (2 + \delta x^2 V_j + i \lambda)$

$$+ \psi_{j-1}^n (-1 + i \delta x g_n)$$

(18)

Eq. (17) then takes the form:

$$\psi_{j+1}^{n+1} (1 + i \delta x g_n) + \psi_j^{n+1} (-2 - \delta x^2 V_j + i \lambda)$$

$$+ \psi_{j-1}^{n+1} (-1 - i \delta x g_n) = \Omega^n_j$$

(19)

The above equation can be solved with the ansatz (1):

$$\psi_{j+1}^{n+1} = e_j^n \psi_j^{n+1} + f_j^n$$

(20)

Which yields expressions for the quantities $e_j^n$ and $f_j^n$:

$$e_j^n = \frac{1 - i \delta x g_n}{1 + i \delta x g_n \psi_{j-1}^{n+1}} + \frac{2 + \delta x^2 V_j - i \lambda}{1 + i \delta x g_n} a$$

$$f_j^n = \frac{1 - i \delta x g_n}{1 + i \delta x g_n \psi_{j-1}^{n+1}} + \frac{\Omega_j^n}{1 + i \delta x g_n} b$$

(21)

(22)

Boundary conditions for the above quantities are now 
needed. These are obtained from the boundary condition 
on the wave function ($\psi_0^n = \psi_{J+1}^n = 0$ for all $n$):

$$\psi_0^{n+1} = \frac{2 + \delta x^2 V_j - i \lambda}{1 + i \delta x g_n} \psi_0^{n+1} + \frac{\Omega_{j-1}^n}{1 + i \delta x g_n} \psi_{j-1}^{n+1}$$

(23)

which in turn implies
Using Eqs. (21a–21b), one can now obtain $e_j^n$ for $j = 2, \ldots, J - 1$. Similarly, the boundary condition for $\psi_{j-1}^{n+1}$ yields:

$$\psi_{j-1}^{n+1} = -f_{j-1}^n/e_{j-1}^n$$

One can now update the wave function for $j = J - 2, \ldots, 2$ using the ansatz of Eq. (21):

$$\psi_j^{n+1} = (\psi_{j+1}^{n+1} - f_j^n)/e_j^n$$

which completes the numerical scheme.

I now apply this method to a specific example. It has long been known [5] for a two level system that if a harmonic perturbation is applied such that the excitation frequency matches approximately the spacing between quasi levels, which have a finite lifetime in the well. However, due to the finite width of the barrier separating the well region from the free region, the excited states become quasi-levels, which have a finite lifetime in the well. In the numerical calculations which follow, we have adjusted the height of the barrier such that only one quasi level is present among $\sim 100$ “continuum states”. By applying a dipole field on this system, with a frequency which corresponds to the spacing between the ground state and a quasi level, the wave function of a particle, initially in the ground state, will make transitions to the quasi level, and consequently leak out in the free region if the barrier is not too thick. The current generated in the free region then depends on the amplitude and frequency of the driving field, as well as the characteristics of the barrier.

Typical values for the parameters of the potential of Fig. 3 are $a = 4$, $b = 2$, $c = 200$, $V = 1$, $W = 3$. The bound and excited states wave functions are specified by the connection formulas for the wave functions at each boundary, and the corresponding energies of these states are determined numerically. To determine the energy of the quasi levels, the integrated density in the well region for all states with $E > 0$ is calculated, and the level for which this quantity is a maximum is selected. Alternatively, all matrix elements of the position operator between the ground and excited states are computed, and the level for which the probability of transition is a maximum is selected. In practice, these two procedures give the same result. Once the spacing between the quasi level energy $E_Q$ and the ground state energy $E_G$ is known, the driving frequency $\omega$ is chosen to correspond to an exact resonance $\omega = E_Q - E_G$, or alternatively, one can include a finite mismatch $\delta \omega$. At $t = 0$, the particle is taken to be in the ground state, and at each time step, the integrated density $\rho_t(t) = \int_a^b dx \rho(x, t)$ in the free region is computed, as well as the overlap $\left|<G|\psi(t)> \right|^2$ with the ground state. The time step has to be chosen small compared to the period of the external field: here, we choose $\delta t = 0.0125 \times (2\pi/\omega)$.

In Fig. 3b, $\rho_t(t)$ is plotted for field amplitude $\epsilon = 0.1$. The barrier width ($b = 2$) and height ($W = 3$) are chosen to be large enough that the “escape time” of the wave function is large compared to other characteristic times of the problem. Moreover, the driving frequency has been chosen to be close to the resonance condition $(\delta \omega/\omega) = 0.0001$, which is smaller than the spacing between “continuum” levels ($E > 0$), in order to check agreement with the two level approximation. The integrated density exhibits steps or plateaux, which allow to identify the Rabi frequency $\omega_R$. Supposed to the plateaux structure are small amplitude oscillations which period corresponds to the driving frequency. As the simulation is started, transitions to the quasi levels and neighboring levels start occurring, but after a period $T_R = 2\pi/\omega_R$, the contribution of the wave function which remained trapped in the well has returned for the most part in the ground state. This is illustrated in fig. 3b : indeed, aside from a slow decay associated with the transparency of the barrier, the overlap with the ground state $\left|<G|\psi(t)> \right|^2$ oscillates with period which matches exactly the plateaux structure. After the first plateau, $\rho_t(t)$ picks up again as the next oscillation returns the trapped wave function to the excited states. Upon doubling/halving the coupling strength, the period of the oscillations is twice as small/large, confirming the fact that the Rabi oscillation frequency scales linearly with the field amplitude if the resonance condition is met. The “measured” Rabi frequency $\omega_R \approx 0.01$ is in reasonable agreement with the two level result $\hbar \omega_R = |<G|x|1>| \epsilon \approx 0.04$. To estimate the magnitude of the matrix element $<G|x|1>$ between the ground state and the quasi level, the parameters of an infinite well were chosen.

The evolution of the wave function for the same pa-
parameters is depicted in Figs. 3a–c for times \( t = 1500 \), \( t = 3000 \), and \( t = 4500 \), where the probability density is plotted as a function of position. The well and barrier region lies on the left hand side of the pictures. The Rabi frequency corresponds roughly to a period \( T_R \sim 1500 \), and the leakage current is small, which explains by most of the wave function remains in the well. At time \( t = 1500 \) (Fig. 3a), a portion of the wave function has been transmitted in the free region, as a Rabi oscillation with the quasi level has been completed. At \( t = 3000 \) (Fig. 3b), the system has undergone two Rabi oscillations and another wave packet escapes from the well, and similarly for \( t = 4500 \) (Fig. 3c) after three oscillations. The wave function is therefore emitted by “bursts” out of the well every time a Rabi oscillation is completed.

In summary, a method has been described, which simulates the quantum evolution of a particle in a square barrier/well potential, in the presence of a dipole field. Using a gauge transformation, a Hamiltonian which terms commute with each other is obtained, which in turns allows to write an exact expression for the evolution operator. Using a generalization of the finite difference scheme of (GSS), the time evolution is obtained. This method is particularly useful to model activation/tunneling processes for nano structures exposed to an external microwave field. As an example, it is possible to use the two state slow (Rabi) oscillations of a two level system to build a switching device. The device is composed of a well region separated from a continuum region by a barrier. The activation of the ground state to a quasi level using microwave frequencies allows to generate a current in the free region in a controllable manner. More details on the characteristics of this device will be provided elsewhere.

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* Present address: Institut Laue–Langevin, BP 156, 38042 Grenoble, France.
[1] A. Goldberg, H. Schey, and J.L. Schwartz, Am. J. Phys. 35, 177 (1967).
[2] G. Baym, Lectures on Quantum Mechanics, (Addison Wesley, New York).
[3] D. L. Haavig and R. Reifenberger, Phys. Rev. B 26, 6408 (1982).
[4] E. E. Mendez, in Physics and Applications of Quantum Wells and Superlattices, E.E. Mendez and K. von Klitzing eds., (Plenum, New York 1987).
[5] L.D. Landau and E.M. Lifshitz, Quantum Mechanics, (Pergamon, New York 1963).
[6] Th. Martin and G. Berman, preprint (1994).