TIME-DEPENDENT SCHRÖDINGER EQUATION IN 1D: ONE AND TWO PARTICLES

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1. Why this project ?

Time-dependent quantum phenomena constitute a very important and extremely active area of current research in condensed matter physics. Indeed, an accurate understanding/description of the dynamics of a quantum system is expected to become of great technological interest, since future nanodevices will operate under the influence of ever-faster time-varying external fields. Accordingly, those regarded at present as marginal transient effects in time will soon become center stage features to be considered in device fabrication and performance. A proper theoretical description of time-dependent quantum phenomena is a rather challenging task. Often, the main difficulty is to account for the interaction among electrons out of equilibrium. In this project, we consider the two simplest examples of this sort, i.e. the dynamical behavior of one and two electrons in the presence of electron-electron interactions. We confine ourselves to one-dimensional systems. Working with this project, the student will gain an elementary operational knowledge of the time-dependent Schrödinger equation, an additional topic with respect to the contents of the course lectures. Completion of the project consists in performing the two tasks described below.

2. Preliminaries

In the one-dimensional case, the non-relativistic time-dependent Schrödinger equation for one particle reads

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]\psi(x,t) \tag{1}$$

where $V(x,t)$ is a time dependent potential, and the solution must satisfy in time a boundary condition for the initial state $\psi(x,t_0)$. We now proceed to a discretization of the space-coordinate x, and introduce a linear grid of equally spaced points $x_n = n\Delta, n = 0, \pm1, \pm2, \cdots$. This permits us to use a discretized (three-point) version of the second derivative in x, namely

$$f''(x_n) = \frac{f(x_{n+1}) - 2f(x_n) + f(x_{n-1})}{\Delta^2}. \tag{2}$$

Introducing the notation $\psi_n \equiv \psi(x_n)$ we can discretize (in space) the Schrödinger equation as follows:

$$i\hbar\frac{\partial\psi_n(t)}{\partial t} = -\frac{\hbar^2}{2m\Delta^2}\left[\psi_{n-1}(t) - 2\psi_n(t) + \psi_{n-1}(t)\right] + V_n(t)\psi_n(t). \tag{3}$$

We can go further and i) start to consider directly a discrete system, ii) move to the ket-bra Dirac's notation iii) set $\hbar = 1$, so that we can write

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle, \tag{4}$$

where

$$\hat{H}(t) = V\sum_n(|n\rangle\langle n+1| + h.c.) + \sum_n \epsilon_n(t)|n\rangle\langle n|. \tag{5}$$

In Eq.(4), $V = -\frac{1}{2m\Delta^2}$ (since $\hbar = 1$) and $\epsilon_n(t) = V(x_n, t) + \frac{1}{m\Delta^2}$. We can easily convince ourselves that Eq.(4) is just a re-write of Eq.(3), if we i) multiply both sides of Eq.(4) from the left with $\langle n|$, ii) use the expression of $\hat{H}$ in Eq.(5), and iii) take into account that $\psi_n(t) \equiv \langle n|\psi(t)\rangle$. As a final adjustment, we note that the site-label n runs over all integer values (as a results of our discretization of the x-axis). However, to do some practical calculations within time-dependent quantum-mechanics, we will restrict n to a finite (and smal)l set of L values , i.e. $1 \leq n \leq L$. With this prescriptions, we finally arrive at

$$|\psi(t)\rangle = \sum_{n=1}^{L}\psi_n(t)|n\rangle, \quad i\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle, \quad \langle n|m\rangle = \delta_{nm} \tag{6}$$

$$\hat{H}(t) = V\sum_{n=1}^{L-1}(|n\rangle\langle n+1| + h.c.) + \sum_{n=1}^{L}\epsilon_n(t)|n\rangle\langle n|. \tag{7}$$

We are now looking at the dynamics of a particle (e.g. an electron) which moves ("hops") along the "sites" n of a 1D chain of length L, with hopping amplitude V and time-dependent "onsite" energies $\epsilon_n(t)$. The set of states $\{|1\rangle, \cdots |L\rangle\}$ constitutes a complete basis set for any quantum state of particle in the chain with L sites. We can in fact forget where this simple model Hamiltonian was originating from, and consider this as a quantum mechanical problem on its own, where the parameters in $\hat{H}$, i.e. $V, \epsilon_n(t)$ can be chosen independently from the corresponding original problem of Eq.(1). This preliminary discussion provides the layout for a description of the project.

3. The project

Let us consider the system described by Eqs.(6,7), in the special case when $\epsilon_n(t) = \theta(t)\epsilon_1\delta_{n,1}$. That is,

$$\hat{H}(t \leq 0) \equiv \hat{H}_0 = V\sum_{n=1}^{L-1}(|n\rangle\langle n+1| + h.c.). \tag{8}$$

$$\hat{H}(t > 0) \equiv \hat{H}' = H_0 + \epsilon_1|1\rangle\langle 1|. \tag{9}$$

For $t > 0$ we have suddenly added a constant perturbation at the first site of the chain. For this special case, one can explicitly write the solution to Eq.(6):

$$|\psi(t)\rangle = e^{-i\hat{H}'t}|\psi(0)\rangle, \tag{10}$$

where $|\psi(0)\rangle$ is the ground (and initial) state of the system with Hamiltonian $\hat{H}_0$, i.e.

$$\hat{H}_0|\psi(0)\rangle = E_0|\psi(0)\rangle. \tag{11}$$

To find $|\psi(0\rangle)$ in the $|n\rangle$ basis, one needs to diagonalize the $L \times L$ Hamiltonian

$$\begin{pmatrix} 0 & V & 0 & 0 & 0 \\ V & 0 & V & 0 & 0 \\ 0 & V & 0 & \ddots & 0 \\ 0 & 0 & \ddots & 0 & V \\ 0 & 0 & 0 & V & 0 \end{pmatrix} \tag{12}$$

and to choose the state $|\psi(0)\rangle = \sum_{n=1}^{L} \psi_n^0 \, |n\rangle$ with the lowest energy E_0. In the ground state, the particle density at the n-th site is given by $|\psi_n^0|^2$. However, the particle density will change in time for $t > 0$ due to the presence of the perturbation $\epsilon_1|1\rangle\langle 1|$ in $\hat{H}'$. The particle density at site n is defined as $\rho_n(t) = |\psi_n(t)|^2$. It can also be calculated using the operator $\hat{\rho}_n \stackrel{\text{def}}{=} |n\rangle\langle n|$:

$$\rho_n(t) = \langle\psi(t)|\hat{\rho}_n|\psi(t)\rangle. \tag{13}$$

To obtain $\psi_n(t)$ (and thus $\rho_n(t)$), we multiply from the left both sides of Eq.(10) by $\langle n|$:

$$\psi_n(t) = \langle n|\psi(t)\rangle = \langle n|e^{-i\hat{H}'t}|\psi(0)\rangle. \tag{14}$$

To compute the RHS of Eq.(14), we consider all the eigenvalues E_λ and eigenvectors $|\lambda\rangle$ of H' (they satisfy $\hat{H}'|\lambda\rangle = E_\lambda|\lambda\rangle$). Since $\sum_\lambda |\lambda\rangle\langle\lambda| = 1$ (this is the completeness relation for the eigenstates of $\hat{H}'$), we can then proceed as follows:

$$\psi_n(t) = \langle n|e^{-i\hat{H}'t}|\psi(0)\rangle = \langle n|e^{-i\hat{H}'t}\sum_\lambda |\lambda\rangle\langle\lambda|\psi(0)\rangle = \sum_\lambda e^{-iE_\lambda t}\langle n|\lambda\rangle\langle\lambda|\psi(0)\rangle. \tag{15}$$

Since $|\lambda\rangle = \sum_n \psi_n^\lambda |n\rangle$, we finally have

$$\psi_n(t) = \sum_\lambda e^{-iE_\lambda t}\psi_n^\lambda \left[\sum_n \psi_n^\lambda \psi_n^0\right]. \tag{16}$$

TASK 1. Implement numerically Eq.(16), to compute and represent graphically the particle densities $\rho_n(t) = |\psi_n(t)|^2$ for a linear chain of $L = 6$ sites, where $V = -1$ and $\epsilon_1 = \pm 2$. Show the time dependent densities in the time interval $0 \leq t \leq 20$. Discuss the numerical results.

4. Additional preliminaries for the two electron problem

Imagine now that the chain of L sites can accommodate two electrons with opposite spins. For two electrons in the chain, a complete, orthonormal basis set is given by the set of L^2 vectors $\{|n\uparrow; n'\downarrow\rangle\}$, with $1 \leq n \leq L, 1 \leq n' \leq L$. The notation $|n\uparrow; n'\downarrow\rangle$ describes a basis state with one electron with spin-up at site n, and one electron of spin-down at site n'. From now onwards, we shorthand the notation by using $|n; n'\rangle \equiv |n\uparrow; n'\downarrow\rangle$. The two electrons can in principle be anywhere in the chain; the most general 2-electron state $|\Psi_s(t)\rangle$ can be written as

$$|\Psi_2(t)\rangle = \sum_{n=1}^{L}\sum_{n'=1}^{L} \Psi_{nn'}|n; n'\rangle. \tag{17}$$

If the interactions between electrons are not included, the ground state Hamiltonian $H_0^{(2)}$ for the two electrons can be easily written by making use (and slightly generalizing) the notions introduced for the one-electron case. As an example, for two electrons in an $L = 3$ chain, the complete basis set $\{|n; n'\rangle\}$ is explicitly given by

$$|1;1\rangle, |1;2\rangle, |1;3\rangle, |2;1\rangle, |2;2\rangle, |2;3\rangle, |3;1\rangle, |3;2\rangle, |3;3\rangle. \tag{18}$$

Within this basis set, and in the specific order given in Eq.(18), the matrix representation for $H_0^{(2)}$ when the onsite energies are $\epsilon_1, \epsilon_2, \epsilon_3$ is

$$\begin{pmatrix}
2\epsilon_1 & V & 0 & V & 0 & 0 & 0 & 0 & 0 \\
V & \epsilon_1+\epsilon_2 & V & 0 & V & 0 & 0 & 0 & 0 \\
0 & V & \epsilon_1+\epsilon_3 & 0 & 0 & V & 0 & 0 & 0 \\
V & 0 & 0 & \epsilon_1+\epsilon_2 & V & 0 & V & 0 & 0 \\
0 & V & 0 & V & 2\epsilon_2 & V & 0 & V & 0 \\
0 & 0 & V & 0 & V & \epsilon_2+\epsilon_3 & 0 & 0 & V \\
0 & 0 & 0 & V & 0 & 0 & \epsilon_1+\epsilon_3 & V & 0 \\
0 & 0 & 0 & 0 & V & 0 & V & \epsilon_2+\epsilon_3 & V \\
0 & 0 & 0 & 0 & 0 & V & 0 & V & 2\epsilon_3
\end{pmatrix}. \tag{19}$$

We now introduce the interactions among electrons. To keep things simple, we assume that the electrons interact only when they are at the same site, i.e. the interaction term is

$$\sum_n U_n |n; n\rangle\langle n; n|. \tag{20}$$

For the $L = 3$ case, in the presence of the interactions, the matrix for $H_0^{(2)}$ becomes

(21)
$$\begin{pmatrix} 2\epsilon_1+U_1 & V & 0 & V & 0 & 0 & 0 & 0 & 0 \\ V & \epsilon_1+\epsilon_2 & V & 0 & V & 0 & 0 & 0 & 0 \\ 0 & V & \epsilon_1+\epsilon_3 & 0 & 0 & V & 0 & 0 & 0 \\ V & 0 & 0 & \epsilon_1+\epsilon_2 & V & 0 & V & 0 & 0 \\ 0 & V & 0 & V & 2\epsilon_2+U_2 & V & 0 & V & 0 \\ 0 & 0 & V & 0 & V & \epsilon_2+\epsilon_3 & 0 & 0 & V \\ 0 & 0 & 0 & V & 0 & 0 & \epsilon_1+\epsilon_3 & V & 0 \\ 0 & 0 & 0 & 0 & V & 0 & V & \epsilon_2+\epsilon_3 & V \\ 0 & 0 & 0 & 0 & 0 & V & 0 & V & 2\epsilon_3+U_3 \end{pmatrix}.$$

This matrix $H_0^{(2)}$ can be diagonalized, to find the ground state $|g^{(2)}\rangle$ and its energy $E_g^{(2)}$. One can also determine the ground state density of the spin-up electron (the spin-down density is identical) at all sites n. We can easily convince ourselves that the density $\rho_{n\uparrow}$ is given in this case by $\langle g^{(2)}|\hat{\rho}_{n\uparrow}|g^{(2)}\rangle$, where $\hat{\rho}_{n\uparrow} = \sum_{n'=1}^{L} |n;n'\rangle\langle n;n'|$. A related quantity of interest is the average double occupancy $\rho_n^{(2)}$ at site n. This can be expressed as $\rho_n^{(2)} = \langle g^{(2)}|\hat{\rho}_n^{(2)}|g^{(2)}\rangle$, where $\hat{\rho}_n^{(2)} = |n;n\rangle\langle n;n|$. The double occupancy $\rho_n^{(2)}$ gives a direct measure of the effect of the interaction between electrons. A moment of reflection shows that the inclusion of a sudden onsite perturbation at site $n = 1$ at time $t = 0^+$ simply amounts to change the values of ϵ_1 in Eq.(21). In this way, one can study the time evolution of two electrons in a $L = 3$ chain.

TASK 2. Derive and implement numerically the equivalent of Eq.(16) for the two-particle case for a chain with $L = 6$. For the parameters in the Hamiltonian, we set $U_1 = 0, U_{n>1} = 15$, $V = -1$, $\epsilon_{n>1} = 0$ for all times t. On the other hand, the value of ϵ_1 determines $\hat{H}(t)$ and thus changes in time. For $\hat{H}(t \leq 0)$, we set $\epsilon_1 = -15$. For $t > 0$, different values of ϵ_1 determine different types of dynamics. The aim of Task 2 is to study the time behavior of $\rho_{n\uparrow}$ and $\rho_n^{(2)}$ for $0 \leq t \leq 20$, for different values of ϵ_1.

- Consider the values $\epsilon_1 = 5, 15$. Calculate the dynamics and discuss the results.
- Describe, if any, the qualitative differences between the two cases above.
- For such two cases $\rho_{n\uparrow}$ and $\rho_n^{(2)}$ differ from each other. Can you say why?
- By performing a scan of the values of ϵ_1 for $20 < \epsilon_1 < 25$, determine if there is a value of ϵ_1 for which $\rho_{n\uparrow} \simeq \rho_n^{(2)}$.
- If such regime is found, provide an explanation of why $\rho_{n\uparrow} \simeq \rho_n^{(2)}$.
- What about the different timescales in the particle propagation (through the chain) for the cases considered ?