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PSU-Physics

PH 411/511
Fall-2008

INTRODUCTION TO QUANTUM MECHANICS

Homework - 5

Due: 11-12-2009

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1. The evolution operator $\tilde{U}(t_2, t_1)$ acting on a state $|\Psi\rangle$ at a given time t_1 gives the state at the time t_2. Symbolically,

$$\underbrace{\tilde{U}(t_2,t_1)}_{Operator}\underbrace{|\Psi(t_1)\rangle}_{State} = \underbrace{|\Psi(t_2)\rangle}_{State}$$

Assuming that only 4 base states $\{\,|n\rangle\,;\; n = 1, 2, 3, 4\,\}$ are necessary to completely describe a quantum system:

1.A Construct explicitly the corresponding matrix $[U](t_2,t_1)$ representing the $\tilde{U}(t_2,t_1)$ operator.

1.B Find the form that the matrix $[U](t_2,t_1)$ adopts when $t_2 \to t_1$

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2. Assume that only 4 base states $\{\,|n\rangle\,;\; n = 1, 2, 3, 4\,\}$ are necessary to completely describe a quantum system. That is, a general state $|\Psi(t)\rangle$ can be expressed as $|\Psi(t)\rangle = \sum_{n=1}^{4} |n\rangle A_n(t)$.

We know that, the value of a particular amplitude $A_m(t+\Delta t)$ at the time $t+\Delta t$ can be calculated in terms of the four amplitudes $A_n(t)$ (n = 1, 2, 3 and 4) evaluated at the previous time t. Indeed, for small Δt we have,

$$A_m(t+\Delta t) = \sum_{n=1}^{4}\left(\delta_{mn} - \frac{i}{\hbar}(\Delta t)\, H_{mn}(t)\right)A_n(t)$$

2.A For each value of m (i.e. 1, 2, 3, and 4) evaluate $\sum_{n=1}^{4} \delta_{mn} A_n(t)$

Subsequently, express the result in a matrix format

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Subsequently, express the result in a matrix format

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3. In the ammonia molecule, introduced in section 7.1, we identify two possible states:

State $|1\rangle$ the "down" state (corresponding to a charge distribution when the nitrogen is *below* the plane defined by the three hydrogen atoms.)

State $|2\rangle$ the "up" state (corresponding to a charge distribution when the nitrogen is *above* the plane defined by the three hydrogen atoms.)

The evolution in time of a wavefunction

$$|\psi(t)\rangle = |1\rangle A_1(t) + |2\rangle A_2(t) \qquad (1)$$

is governed by

$$i\hbar\frac{dA_1(t)}{dt} = E_0 A_1 - W A_2$$

$$i\hbar\frac{dA_2(t)}{dt} = -W A_1 + E_0 A_2$$

Let's define the "new" states $|S_I\rangle$ and $|S_{II}\rangle$ in terms of the "old" states $|1\rangle$ and $|2\rangle$ according to:

$$|S_I\rangle \equiv \frac{1}{\sqrt{2}}(\ |1\rangle + |2\rangle\ ) \quad , \quad |S_{II}\rangle \equiv \frac{1}{\sqrt{2}}(\ |1\rangle - |2\rangle\ )$$

In terms of the new states, the wavefunction can also be expressed as

$$|\psi(t)\rangle = |S_{\rm I}\rangle B_{\rm I}(t) + |S_{\rm II}\rangle B_{\rm II}(t) \qquad (2)$$

3A Evaluate $\langle S_I|S_I\rangle$, $\langle S_{II}|S_{II}\rangle$, $\langle S_I|S_{II}\rangle$
(Assume the states $|1\rangle$ and $|2\rangle$ are ortho-normalized.)

3B Express each of the two B-amplitudes in terms of the A-amplitudes

3C Find explicitly $B_I(t)$ and $B_{II}(t)$ .as a function of t, and in terms of E_o and W.

3D Write down the matrix representation of the Hamiltonian operator when using the base {$|1\rangle$, $|2\rangle$ }

Write down the matrix representation of the same Hamiltonian operator but when using the base $\{|S_I\rangle \; , \; |S_{II}\rangle\}$

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4. Dynamics of an electron in a one-dimensional crystal

By assuming that the electron will jump only from one atom to the neighbor of either side (with an amplitude probability equal to $-W$), one arrives to the following Hamiltonian equations.

$$i\hbar \frac{dA_n}{dt} = -W A_{n-1} + E_o A_n - W A_{n+1} \qquad (3)$$

4.1 What is the meaning (or interpretation) of E_o in these equations

4.2 Show that these equations have solutions of the form

$$|\,\phi^{(E)}(t)\,\rangle = \sum_n |\,n\rangle A_n^{(E)}(t) = \sum_n |\,n\rangle\, a_n\, e^{-(i/\hbar)(E)\,t} \qquad (4)$$

What is the meaning of E in this solution (4)

What is the condition to be satisfied by a_n (for (4) to become a solution of Eq. (3))?

What is the physical meaning of a_n in the solution (4)

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5. Dynamics of an electron in a one-dimensional crystal

For the case of a low energy wave-packet whose main wavenumber k is around k_o, show explicitly that

$$m_{eff}\, \mathrm{v}_g = \hbar k_o$$

(in the jargon of solid state physics, $\hbar k$ is called the crystal momentum.)

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6. Dynamics of an electron in a one-dimensional crystal

For a free particle $E(k) = \frac{1}{2m}\hbar^2 k^2$. From this expression, the mass m can be obtained by differentiating $E(k)$ twice. That is,

$$m = \frac{\hbar^2}{\frac{d^2}{dk^2} E(k)}$$

Consider now the case of an electron in a lattice, where

$$E(k) = 2W - 2W \,\mathrm{Cos}(k\,\mathrm{b})$$

6A Use the definition given above to obtain the effective mass m^* associated to an electron in a lattice. That is, evaluate

$$m^* = \frac{\hbar^2}{\frac{d^2}{dk^2} E(k)}$$

6B Evaluate the group velocity of a wavepacket describing the motion of an electron in a lattice

6C Evaluate the product of the effective mass with the group velocity.

Verify that for small values of k (compared to π/b) the product

$$m^* \mathrm{v}_g \xrightarrow[small\ k]{} \hbar k$$