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December 13th, 2023
WS 2023/24

Problem 9.1: Transition probability for a harmonic perturbation [**Oral** | 6 pt(s)]

ID: ex_transition_probablity_for_harmonic_perturbation:aqt2324

Learning objective

To study the structure of molecular and atomic systems, one needs to know how electromagnetic radiation interacts with these systems. We will explore the effect of a time dependent perturbation on the transition probability of the system from one stationary state to another.

Consider a perturbation which depends harmonically on time (i.e., the time between the moments of turning the perturbation on and off):

$$\hat{V}(t) = \hat{v}e^{i\omega t} + \hat{v}^{\dagger}e^{-i\omega t},$$

where $\hat{v}$ is a time-independent operator. This perturbation provokes transitions of the system from one stationary state to another.

a) Using the expression **2**pt(s)

$$P_{if}(t) = \left| -\frac{i}{\hbar}\int_0^t \left\langle \psi_f|\hat{V}(t')|\psi_i\right\rangle e^{i\omega_{fi}t'}dt'\right|^2, \tag{1}$$

and neglecting the cross-terms (i.e. assuming $|a+b|^2 \approx |a|^2 + |b|^2$) derive an expression for the transition probability to this perturbation.

b) Draw a schematic figure, of the transition probability amplitude as a function of ω_{fi} for a fixed time t. What are the maximum values? Describe what it means to have the frequency of the perturbing field close to $\pm\omega_{fi}$. **2**pt(s)

c) Now consider the case where $t \to \infty$, and show that the expression derived above reduces to **2**pt(s)

$$\Gamma_{if} = \frac{2\pi}{\hbar}\left|\langle\psi_f|\hat{v}|\psi_i\rangle\right|^2 \delta\left(E_f - E_i + \hbar\omega\right) + \frac{2\pi}{\hbar}\left|\left\langle\psi_f\left|\hat{v}^{\dagger}\right|\psi_i\right\rangle\right|^2 \delta\left(E_f - E_i - \hbar\omega\right). \tag{2}$$

[Hint: Use the asymptotic relation $[\lim_{t\to\infty}\frac{\sin^2(yt)}{\pi y^2 t} = \delta(y)]$. What are the conditions for the transition rate to be non-zero? Interpret the two kinds of corresponding processes physically.

Problem 9.2: (A)diabatic approximation of potential well [**Oral** | 4 pt(s)]

ID: ex_potential_well_adiabatic_diabatic_approximation:aqt2324

Learning objective

We will see the influence of adiabatic and diabatic changes on the energy spectrum of a particle in a one-dimensional potential well.

A particle is initially $(t<0)$ in the ground state of an infinite, one-dimensional potential well with walls at $x=0$ and $x=a$.

a) If the wall at $x=a$ is moved slowly to $x=8a$, find the energy and wave function of the particle in the new well. Calculate the work done in this process. **2**pt(s)

b) If the wall at $x=a$ is now suddenly moved (at $t=0$) to $x=8a$, calculate the probability of finding the particle in (i) the ground state, (ii) the first excited state, and (iii) the second excited state of the new potential well. **2**pt(s)

Problem 9.3: Adiabatic Approximation and Berry Phase [**Written** | 6 (+3 bonus) pt(s)]

ID: ex_berry_phase_sakurai:aqt2324

Learning objective

In this exercise we will start from general considerations regarding the adiabatic approximation to obtain the so-called Berry phase. This *geometric phase* is particularly important in condensed matter physics and topology. As an example, we will calculate the Berry phase for a spin $1/2$ particle under the influence of a slowly varying in time magnetic field.

We consider the eigenvalue equation

$$H(t)|n;t\rangle = E_n(t)|n;t\rangle, \tag{3}$$

with the index n numbering the states in a certain order and assume that there is no degeneracy. This relation states that at any particular time t, the states and eigenvalues may change. General solutions will be given by the Schrödinger equation of the form

$$i\hbar\frac{\partial}{\partial t}|\alpha;t\rangle = H(t)|\alpha;t\rangle, \tag{4}$$

with

$$\begin{aligned} |\alpha;t\rangle &= \sum_n c_n(t)e^{i\theta_n(t)}|n;t\rangle, \\ \text{where}\quad \theta_n(t) &\equiv -\frac{1}{\hbar}\int_0^t E_n(t')\,dt'. \end{aligned} \tag{5}$$

a) (i) Show that the expansion coefficients in the general solution of the Schrödinger equation (5) can be written as **2**pt(s)

$$\dot{c}_m(t) = -c_m(t)\langle m;t|\left[\frac{\partial}{\partial t}|m;t\rangle\right] - \sum_n c_n(t)e^{i(\theta_n-\theta_m)}\frac{\langle m;t|\dot{H}|n;t\rangle}{E_n-E_m}, \tag{6}$$

Notice that this equation states that as time goes on, states with $n\neq m$ will mix with $|m;t\rangle$ because of the time dependence of the Hamiltonian H, by virtue of the second term.

(ii) Use the adiabatic approximation to show that the solution to (6) will be given by

$$\begin{aligned} & c_n(t) = e^{i\gamma_n(t)} c_n(0) \\ \text{where} \quad & \gamma_n(t) \equiv i \int_0^t \langle n; t'| \left[\frac{\partial}{\partial t'} |n; t'\rangle \right] dt'. \end{aligned} \tag{7}$$

Hint: Consider the effect of equations (6) and (7) on the Schrödinger equation (4) and exploit the orthonormality of the states $\langle m; t|$.

For (ii), consider the time derivative on both sides of eq. (3) and calculate $\langle m; t|\dot{H}|n; t\rangle$.

*b) Assume that the time dependence of the Hamiltonian is represented by a "vector of parameters" $\mathbf{R}(t)$. That is, there exists some space in which the components of a vector $\mathbf{R}(t)$ specify the Hamiltonian and change as a function of time. The eigenvalue equation (3) will be given by $H(t)|n\mathbf{R}(t)\rangle = E_n(\mathbf{R}(t))|n\mathbf{R}(t)\rangle$. **+3pt(s)**

Use this new notation and equation (7) to show that the Berry phase can be rewritten as

$$\begin{aligned} & \gamma_n(C) = \int \mathbf{B}_n(\mathbf{R}) \cdot d\mathbf{a}, \\ \text{where} \quad & \mathbf{B}_n(\mathbf{R}) = i \sum_{m \neq n} \frac{\langle n; t\,|[\nabla_{\mathbf{R}} H]|\, m; t\rangle \times \langle m; t\,|[\nabla_{\mathbf{R}} H]|\, n; t\rangle}{(E_m - E_n)^2}. \end{aligned} \tag{8}$$

where

$$\mathbf{B}_n(\mathbf{R}) = i \sum_{m \neq n} \frac{\langle n; t\,|[\nabla_{\mathbf{R}} H]|\, m; t\rangle \times \langle m; t\,|[\nabla_{\mathbf{R}} H]|\, n; t\rangle}{(E_m - E_n)^2}. \tag{9}$$

Hint: After rewritting the equations in terms of $\mathbf{R}(t)$, use the generalized Stokes' theorem to represent

$$\gamma_n(C) = \oint_C \mathbf{A}_n(\mathbf{R}) \cdot d\mathbf{R} = \int [\nabla_{\mathbf{R}} \times \mathbf{A}_n(\mathbf{R})] \cdot d\mathbf{a}.$$

where $\mathbf{A}_n(\mathbf{R}) \equiv i\langle n; t|\,[\nabla_{\mathbf{R}}|n; t\rangle]$.

To obtain (9), use vector calculus identities and that $|m; t\rangle$ constitutes a complete set of states in $\mathbf{B}_n(\mathbf{R}) \equiv \nabla_{\mathbf{R}} \times \mathbf{A}_n(\mathbf{R})$.

As a particular example on how to use equation (8), we shall consider a spin $1/2$ particle under the influence of a magnetic field. Considering a magnetic moment μ, the Hamiltonian will be given by

$$H(t) = H(\mathbf{R}(t)) = -\frac{2\mu}{\hbar} \mathbf{S} \cdot \mathbf{R}(t), \tag{10}$$

where the magnetic field is represented by a slowly changing vector of parameters $\mathbf{R}(t)$, and $\mathbf{S}$ is the spin $1/2$ angular momentum operator.

c) Show that that the two energy eigenvalues for (10) are given by **2pt(s)**

$$E_{\pm}(t) = \mp \mu R(t),$$

where $R(t)$ is the magnitude of the magnetic-field vector, and the spin-up (down) eigenstates (with respect to the direction of $\mathbf{R}(t)$) are $|\pm; t\rangle$.

Hint: Show it explicitly or by exploiting the rotational symmetry in the system.

d) Finally, show that the Berry's Phase will be given by **2**pt(s)

$$\gamma_{\pm}(C) = \mp\frac{1}{2}\int\frac{\hat{\mathbf{R}}\cdot d\mathbf{a}}{R^2} = \mp\frac{1}{2}\Omega, \tag{11}$$

where Ω is the "solid angle" subtended by the path through which the parameter vector $\mathbf{R}(t)$ travels, relative to an origin $\mathbf{R} = 0$ that is the source point for the field B.

Observe that this emphasizes the "geometric" character of Berry's Phase. Specifics of the path do not matter, so long as the solid angle subtended by the path is the same. The result is also independent of the magnetic moment μ.

Hint: Use the ladder operators $S_{\pm} = S_x \pm iS_y$ to rewrite the x and y components of **S** in terms of S_+ and S_-. Now, consider this new expression and that $S_{\pm}|s,m\rangle = \sqrt{(s \mp m)(s \pm m + 1)}\hbar|s, m\pm 1\rangle$ to evaluate the expressions of the form $\langle\pm;t|\mathbf{S}|\mp;t\rangle \times \langle\mp;t|\mathbf{S}|\pm;t\rangle$.