ECE 5390/MSE 5472, Fall Semester 2015
Quantum Transport in Electron Devices & Novel Materials

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Assignment 4

Policy on assignments: Please turn them in by 5pm of the due date. The due date for this assignment is **Friday, Oct 23rd, 2015**.

General notes: Present your solutions *neatly*. Do not turn in rough unreadable worksheets - learn to **take pride in your presentation**. Show the relevant steps, so that partial points can be awarded. BOX your final answers. Draw figures wherever necessary. Please print out this question sheet and staple to the top of your homework. Write your name and email address on the cover. Some problems may lead to publishable results - be on the lookout!

Problem 4.1) Tunneling escape times by Fermi's golden rule

Recall problem **3.3** in the last assignment, where you solved for the tunneling escape time of a quasi-bound electron. You had to invoke semi-classical arguments to estimate the tunneling escape time there. Now try solving the *same* problem using Fermi's golden rule. Model the problem carefully so that you can apply Fermi's golden rule. Discuss your approximations and their validity.

Problem 4.2) Higher-order time-dependent perturbation theory: Dyson series and diagrams

In class, we used the *interaction representation* to write the perturbed quantum state at time t as $|\psi_t\rangle = e^{-i\frac{H_0}{\hbar}t}|\psi(t)\rangle$, where H_0 is the unperturbed Hamiltonian *operator*. This step helped us recast the time-dependent Schrodinger equation $i\hbar\frac{\partial}{\partial t}|\psi_t\rangle = (H_0 + W_t)|\psi_t\rangle$ to the simpler form $i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = W(t)|\psi(t)\rangle$, where $W(t) = e^{+i\frac{H_0}{\hbar}t}W_t e^{-i\frac{H_0}{\hbar}t}$ is the time-evolution operator. This equation was integrated over time to yield the Dyson series

$$\begin{aligned}|\psi(t)\rangle = \underbrace{|0\rangle}_{|\psi(t)\rangle^{(0)}} + \underbrace{\frac{1}{i\hbar}\int_{t_0}^{t} dt' W(t')|0\rangle}_{|\psi(t)\rangle^{(1)}} + \underbrace{\frac{1}{(i\hbar)^2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' W(t')W(t'')|0\rangle}_{|\psi(t)\rangle^{(2)}} \\ + \underbrace{\frac{1}{(i\hbar)^3}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \int_{t_0}^{t''} dt''' W(t')W(t'')W(t''')|0\rangle}_{|\psi(t)\rangle^{(3)}} + \ldots,\end{aligned} \tag{1}$$

where $|\psi(t_0)\rangle = |0\rangle$ is the initial state. Restricting the Dyson series to the 1st order term in W for a perturbation of the the form $W_t = e^{\eta t}W(r)$, we derived Fermi's golden rule for the transition rate $\Gamma^{(1)}_{0\to n} = \frac{2\pi}{\hbar}|\langle n|W(r)|0\rangle|^2\delta(\epsilon_0 - \epsilon_n)$. We used the relation $\lim_{\eta\to 0^+}\frac{2\eta}{x^2+\eta^2} = 2\pi\delta(x)$ in this process.

(a) Show that the second and third order terms in W in the Dyson series lead to a modified golden rule result

$$\Gamma_{0\to n} = \frac{2\pi}{\hbar}|\langle n|W|0\rangle + \sum_m \frac{\langle n|W|m\rangle\langle m|W|0\rangle}{\epsilon_0 - \epsilon_m + i\eta\hbar} + \sum_{k,l} \frac{\langle n|W|k\rangle\langle k|W|l\rangle\langle l|V|0\rangle}{(\epsilon_0 - \epsilon_k + 2i\eta\hbar)(\epsilon_0 - \epsilon_l + i\eta\hbar)} + ...|^2 \delta(\epsilon_0 - \epsilon_n), \tag{2}$$

where in the end we take $\eta \to 0^+$. We identify the Green's function propagators of the form $G = \sum_m \frac{|m\rangle\langle m|}{\epsilon_0 - \epsilon_m + i\eta\hbar}$. Thus, the result to higher orders may be written in the compact form

$$\Gamma_{0\to n} = \frac{2\pi}{\hbar}|\langle n|W + WGW + WGWGW + ...|0\rangle|^2 \delta(\epsilon_0 - \epsilon_n). \tag{3}$$

(b) Sketch the 'Feynman' diagrams[1] corresponding to the terms in the series, showing the *virtual* states explicitly for the higher order terms.

Problem 4.3) Application of 1st and higher order perturbation theories

5.23 A one-dimensional harmonic oscillator is in its ground state for $t < 0$. For $t \geq 0$ it is subjected to a time-dependent but spatially uniform *force* (not potential!) in the x-direction,

$$F(t) = F_0 e^{-t/\tau}.$$

(a) Using time-dependent perturbation theory to first order, obtain the probability of finding the oscillator in its first excited state for $t > 0$. Show that the $t \to \infty$ (τ finite) limit of your expression is independent of time. Is this reasonable or surprising?

(b) Can we find higher excited states? You may use

$$\langle n'|x|n\rangle = \sqrt{\hbar/2m\omega}(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}).$$

Figure 1: Harmonic oscillator perturbed by a time-dependent field.

Solve this problem from Sakurai (Modern Quantum Mechanics). Note that for part (b), you will need to invoke higher-order perturbation terms as discussed in Problem 4.2.

Problem 4.4) The Boltzmann Transport Equation

In class, we discussed the Boltzmann transport equation

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{r}} f + \mathbf{F}\cdot\nabla_{\mathbf{p}} f = \hat{C} f \tag{4}$$

where the symbols have the usual meanings. The collision term on the right is

$$\hat{C} f = \sum_{k'} [S(k' \to k) f_{k'}(1 - f_k) - S(k \to k') f_k (1 - f_{k'})], \tag{5}$$

where $S(k \to k') = \frac{2\pi}{\hbar}|\langle k'|W(r)|k\rangle|^2 \delta(E_{k'} - E_k \pm \hbar\omega)$ are the scattering rates given by Fermi's golden rule. In this problem, we discuss a few details of this recipe of solving diffusive transport

[1] More accurately, Goldstone diagrams.

problems. For *any* scattering potential, we found that $\frac{S(k \to k')}{S(k' \to k)} = \exp(\frac{E_k - E_{k'}}{kT})$, which led us to distinguish between elastic and inelastic scattering events.

a) Under what conditions can we make the relaxation time approximation (RTA), where $\hat{C}f \approx -(f - f_0)/\tau$? Discuss for both elastic and inelastic scattering events.

b) Outline how from the RTA of the distribution function f, one may obtain charge transport properties such as the electrical conductivity, and thermoelectric properties.

c) For a force $\mathbf{F} = q\mathbf{F_e}$ due to an electric field *alone*, the RTA solution of the BTE took the form

$$f \approx f_0 + \tau(-\frac{\partial f_0}{\partial E})\mathbf{v} \cdot \mathbf{F}. \tag{6}$$

However, in the presence of a crossed electric and magnetic field, the net force is the Lorentz force, $\mathbf{F} = q(\mathbf{F_e} + \mathbf{v} \cdot \mathbf{B})$. Work out a solution for f in the RTA for this situation. You may refer to Wolfe/Holonyak/Stillman's book on the Physics of Semiconductors for this part. Realize that this is the situation encountered in a Hall-effect measurement.

d) Outline how magnetoresistance properties may be obtained from the BTE from your discussion above.

Problem 4.5) Application of Fermi's Golden Rule: Scattering rates due to Point Defects

Assume that in a 3D semiconductor crystal of GaN (electron effective mass = $m^\star \sim 0.2m_0$), point defects of volume density $n_{imp} = N_{imp}/V$ are present. Also, assume that the perturbation V_0 to the crystal potential due to each point defect is confined to a radius R_0 around its location, i.e.,

$$W(\mathbf{r}) = V_0\theta(R_0 - |\mathbf{r}|), \tag{7}$$

where $\theta(...)$ is the unit-step function. This is an example of what is called 'short-range' scatterer.

a) Find the matrix element for scattering of electrons by all the point defects.

b) Assume the single-electron picture, and a parabolic bandstructure. Find an expression for the *momentum* scattering rate $1/\tau_m(E)$ of an electron due to the point defects as a function of its energy above the conduction band edge ($\epsilon = E - E_c$). Make necessary assumptions in the process.

c) Plot the mobility for 'thermal' electrons with $\epsilon = E - E_c \sim k_B T$ at 300 K, as a function of the impurity density in the range $n_{imp} = 10^{15} \to 10^{20}/\text{cm}^3$ for various values of $V_0 = 0.1, 0.3, 0.5, 2.1$ eV. Assume an $R_0 \sim c/4$, where $c \sim 0.51$ nm is the c-axis lattice constant of GaN.

d) This is a reasonable model for things such as alloy scattering, for example, for charge transport of electrons in AlGaN and InGaN layers. Explain why an disordered alloy can be considered to be a perfect crystal with a high density of point defects. Then, estimate the mobility for electrons in $Al_xGa_{1-x}N$ layers as a function of the alloy composition x, by using your results in part (c). Find any references where this might have been done.