

PHYS 622: Quantum Mechanics II
Due date: Tuesday, April 16, 2013

Problem Set #8

Sakurai and Napolitano problems
7.5 [6.4], 7.8 [6.6], 7.9 [6.7]

The old (red) Sakurai (revised, 1st ed.) problems are listed in brackets.

1. Tight binding model of Bloch oscillations

Consider the Hamiltonian for an electron in a 1D periodic potential with lattice spacing $\Delta x = a$ in the tight binding approximation. We will number the lattice sites with the number n and the wavefunction of an electron centered on lattice site n by $|n\rangle$. We will denote the site energy U_0 and the nearest neighbor tunneling energy $-A$. We will assume that the $|n\rangle$ states form a complete basis (e.g. $\langle m|n\rangle = \delta_{mn}$). We now add a constant electric field E directed along the $+x$ -axis.

- Calculate the difference in electric potential energy ΔU_E between two adjacent lattice sites due to the external electric field. Incorporate the external electric field into the tight binding model and write down the Hamiltonian in matrix form in the $\{|n\rangle\}$ basis.
- You will now treat the nearest neighbor tunneling/coupling part of the Hamiltonian as a perturbation of the remaining diagonal terms. Calculate the correction to the energy to second order and the correction to the eigenstates to first order. What is the requirement on A , U_0 , E , and a so that this perturbative treatment is valid?
- Consider an electron in an unperturbed $|\psi\rangle = |n\rangle$ state at $t=0$. Calculate the probability $P_{|n\rangle}(t)$ to be in the $|n\rangle$ state to order $(A/\Delta U_E)^2$ and determine the Bloch oscillation frequency.

2. Wannier states

In this problem you will show that within a given energy band one can construct a basis of states $\{|n\rangle\}$, or Wannier states (sometimes called Wannier-Stark states), that are centered on the lattice sites. We will work in 1D though the results can be generalized to 3D. The Wannier state, $w(x-x_n)$, centered on the n^{th} lattice site at $x=x_n$ is defined in terms of the Bloch states $\psi_k(x)$ of the same band as

$$w(x-x_n) = \frac{1}{\sqrt{N}} \sum_k e^{-ikx_n} \psi_k(x)$$

Here k is the quasi-momentum, N is the number of lattice sites and is assumed to be very large, and the Bloch states are defined as

$$\psi_k(x) = \frac{1}{\sqrt{N}} e^{ikx} u_0(x),$$

where $u_0(x)$ is a lattice potential specific periodic function with the same period as the lattice spacing a , such that $u_0(x+a)=u_0(x)$.

a) Show that the Wannier states centered on two different lattice sites m and n are orthogonal:

$$\int w^*(x - x_n) w(x - x_m) dx = 0, \quad n \neq m$$

b) The Wannier states are centered on the n th lattice site at $x=x_n$. Show that the Wannier states have the form

$$w(x - x_n) = \frac{\sin(\pi(x - x_n)/a)}{\pi(x - x_n)/a} u_0(x)$$