HOME WORK #3

(due date: Monday, 8 October 2007)

1. Consider a spin-less particle inside a one-dimensional potential well $V_0(x)$:

$$V_0(x) = \begin{cases} 0 & (|x| < a) \\ +\infty & (|x| > a) \end{cases}$$

(a) Find the eigenvalues $\{E_n^0\}$ and eigenfunctions $\{u_n^0(x)\}$ of the Hamiltonian $\mathscr{H}_0$:

$$\mathscr{H}_0 = p^2/2m + V_0(x).$$

Now let us consider an additional delta-function potential term at $x = 0$,

$$\mathscr{H}_1(\lambda) = \frac{\hbar^2}{2ma}\lambda\delta(x),$$

where λ ranges from $-\infty$ to $+\infty$.

(b) Assuming $|\lambda| \ll 1$, calculate the energy corrections $\Delta\varepsilon_n$ to the first order in λ and show that the solutions of $\mathscr{H}(\lambda) = \mathscr{H}_0 + \mathscr{H}_1(\lambda)$ approach to those of (a) as $\lambda \to 0$.

(c) Working out an exact solution of the Hamiltonian $\mathscr{H}(\lambda)$, show that there exists a negative energy solution, which does not correspond to any state of $\mathscr{H}_0$. Discuss whether it is possible to describe this negative energy state in terms of $\{u_n^0(x)\}$.

It is easy to find a complete set of states for the Hamiltonian $\mathscr{H}$ in the limit of $\lambda \to \infty$, i.e., $\mathscr{H}(\lambda = \infty)$.

(d) Would it be possible to describe the solutions $\{E_n^0\}$ and $\{u_n^0(x)\}$ of $\mathscr{H}_0$ or $\mathscr{H}(\lambda < \infty)$ starting from the solutions of $\mathscr{H}(\lambda = \infty)$?

2. Consider a 1-D Kronig-Penny potential with δ-functions of strength λ,

$$V(\lambda) = \lambda \sum_{n=1}^{N} \delta(x - na),$$

where the entire "crystal" has a period of Na, i.e., $V(x) = V(x + Na)$.

(a) The potential $V(\lambda)$ can be represented in a Fourier series form:

$$V(\lambda) = \lambda \sum_{n=1}^{N} \delta(x-na) = \sum_m V_m \exp\left[i\left(\frac{2\pi m}{a}\right)x\right]$$

Obtain V_m in terms of λ.

(b) Using a periodic boundary condition $\psi(x) = \psi(x + Na)$, we can find a complete set of solutions for the zeroth-order, i.e., free particle, Hamiltonian $\mathscr{H}_0 = p^2/2m$. When we apply the second-order perturbation theory to $V(\lambda)$, show that the non-degenerate perturbation theory breaks down when the free electron momentum k matches the condition $|k| = m(\pi/a)$ (m is a positive integer).

(c) When $|k| \neq m(\pi/a)$, one can apply the second-order perturbation theory to find the eigenvalues. Compare the second order corrections to those of the exact solutions, which you may find in the usual QM textbook. For example, see pp. 99–103 in Quantum Physics by Gasiorowicz.

(d) Apply the degenerate perturbation theory to estimate the widths of the forbidden gaps in the energy bands of the periodic potential. Compare the results with those of the exact solutions.