6.730 PHYSICS FOR SOLID STATE APPLICATIONS

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PROBLEM SET 1

Issued: 2-7-96 Due: 2-14-96, at the beginning of class.

Readings:
Sentury, 6.730 Course Notes, Chapter 1.
Aschroft and Mermin: Chapters 19 and 20.
Hagelstein: H_2^+ molecular ion (review).

Problem 1.0
Please send your email address to TA: binx@mit.edu.

Problem 1.1 Delta function potential (Quantum mechanics review problem).
Consider a potential that can be modeled as $V(x) = -v_0\delta(x)$ where v_0 is positive.

(a) Show that the boundary conditions on $\psi(x)$ are
  i. $\psi(x)$ is continuous at $x = 0$,
  ii. $\left.\frac{d\psi}{dx}\right|_{0^+} - \left.\frac{d\psi}{dx}\right|_{0^-} = \frac{-2mv_0}{\hbar^2}\psi(0)$.

(b) For $E < 0$, show that there exists a bound state such that $\lim_{x\to\pm\infty} \psi(x) = 0$. Find the wave function and the energy.

(c) For $E > 0$, show that if a particle is incident from the left that

$$\begin{aligned} \psi_1(x) &= Ae^{ikx} + Be^{-ikx} \qquad x \le 0 \\ \psi_2(x) &= Ce^{ikx} \qquad x \ge 0 \end{aligned}$$

Find the reflection and transmission coefficients.

Problem 1.2 Delta function molecular ion.
A single electron is bound between two delta function potentials so that the total potential is

$$V(x) = -v_o\left[\delta(x-a) + \delta(x+a)\right]$$

Let a trial wavefunction be given as

$$\Psi(x) = C\left[\phi(x-a) + \phi(x+a)\right]$$

where C is the normalization constant. Also $\phi(x)$ is the bound state solution for an electron in a single delta-function potential $-v_o\delta(x)$; namely

$$\phi(x) = \sqrt{\kappa}e^{-\kappa|x|}$$

where $\kappa = mv_o/\hbar^2$ and the ground state energy is $E_o = -mv_o^2/2\hbar^2$.

(a) Find the normalization constant C.

(b) Show that the total energy of the state Ψ is given by

$$E = E_o + \frac{\langle\phi_1|V_2|\phi_1\rangle + \langle\phi_1|V_1|\phi_2\rangle}{1 + \langle\phi_1|\phi_2\rangle}.$$

Here $\langle\phi_1|V_2|\phi_2\rangle = \int \phi(x-a)V(x+a)\phi(x+a)\,dx$. Evaluate E in terms of E_o and κ and a.

(c) If $\kappa a \gg 1$ what is the dominate correction to the energy? Explain the origin of this term.

(d) What is the energy for $\kappa a \ll 1$. Explain why this gives an incorrect answer.

Problem 1.3 Molecular crystals.

Use Matlab to numerically evaluate the lattice sums A_6 and A_{12} for a cubic and face-centered cubic lattice, and compare your results with Table 20.2 in Aschcroft and Mermin. Attach your .m files.

Problem 1.4 Finite Basis Set Expansion.

Given an hermitian hamiltonian $\hat{\mathcal{H}}$, and a set of N orthogonal basis functions $|\phi_n\rangle$ (such that $\langle\phi_n|\phi_m\rangle = \delta_{nm}$), show that the best available estimation for the energies and the wavefunctions of the form $\psi = \sum_{n=1}^{N} c_n\phi_n$ is obtained from the eigen values and the eigen vectors of the matrix $\mathcal{H}_{nm} = \langle\phi_n|\hat{\mathcal{H}}|\phi_m\rangle$. Assume that the best estimation is one which minimizes the expectation value of the energy with repect to the c_n's. (See Morrison *et al.*, *Understanding More Quantum Physics*, pp. 99—101 for guidance if you need a hint.)