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Exercise Set 9

(Due date: Tuesday, January 12, 2010)

Exercise 19 (**Kronig Penney model in tight binding approximation**) (20 points)

Solve the Kronig Penney model from Exercise 17 in tight binding approximation.

a) First solve the "atomic problem" (only a single attractive delta potential) exactly.

b) Now calculate the overlap matrix elements of the "atomic" wave functions of the bound state explicitly. Compare the result for the bandstructure with the exact result from Exercise 17.

Exercise 20 (**Tight binding approximation and van-Hove singularities**) (15 points)

a) Calculate the energy dispersion $\varepsilon(\vec{k})$ in tight binding approximation, considering hopping only between nearest neighbors for

- a body centered cubic (bcc) lattice with primitive vectors

$$\vec{a}_1 = \frac{a}{2}\begin{pmatrix}-1\\1\\1\end{pmatrix},\ \vec{a}_2 = \frac{a}{2}\begin{pmatrix}1\\-1\\1\end{pmatrix},\ \vec{a}_3 = \frac{a}{2}\begin{pmatrix}1\\1\\-1\end{pmatrix},$$

  where a is the lattice constant, and
- a face centered cubic (fcc) lattice with primitive vectors

$$\vec{a}_1 = \frac{a}{2}\begin{pmatrix}1\\1\\0\end{pmatrix},\ \vec{a}_2 = \frac{a}{2}\begin{pmatrix}1\\0\\1\end{pmatrix},\ \vec{a}_3 = \frac{a}{2}\begin{pmatrix}0\\1\\1\end{pmatrix}.$$

b) The density of states can be written, as in the case of the phonon density of states, as a surface integral over surfaces of constant ε:

$$\rho(\varepsilon) = \frac{1}{N}\sum_{n\vec{k}} \delta\big(\varepsilon - \varepsilon_n(\vec{k})\big) = \frac{V}{N}\frac{1}{4\pi^3}\sum_n \int_{S(\varepsilon)} \frac{ds}{\left|\nabla_{\vec{k}}\varepsilon_n(\vec{k})\right|},$$

where $S(\varepsilon)$ is the surface in $\vec{k}$ space that is defined by $\varepsilon = \varepsilon(\vec{k})$, and ds is the corresponding surface element. For energies for which the dispersion relations $\varepsilon_n(\vec{k})$ have a horizontal tangent, *i.e.* they fulfil $\nabla_{\vec{k}}\varepsilon_n(\vec{k}) = 0$, singularities called van-Hove singularities appear in the density of states. Consider the dispersion relations for the nearest neighbor tight binding model determined in a). At which energies do you expect van-Hove singularities?