SYip
5/11/05

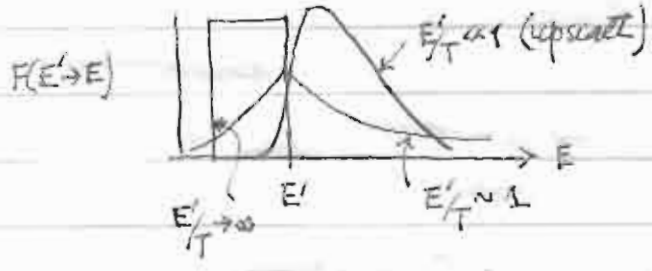
22.106 Spring 2005 Quiz Solutions (sketch)

Prob 1

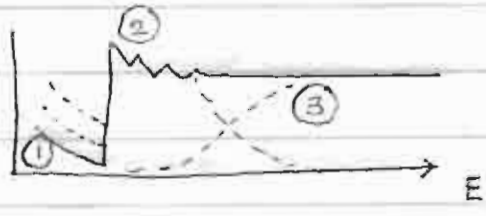
(a) theoretical c.x. is a function of relative speed, to obtain $F(E'\to E)$ we need to average over target nuclear velocity,

$$\sigma_{eff}(v') \sim \int |\underline{v}'-\underline{V}|\, \sigma_{theo}(|\underline{v}'-\underline{V}|)\, P(V,T)\, d^3V \rightarrow \text{a function of } E'/k_BT$$

Maxwellian



(b)



① phonon absorption (T-dep)
② Bragg reflection (T-indep)
③ phonon emission (T-indep)

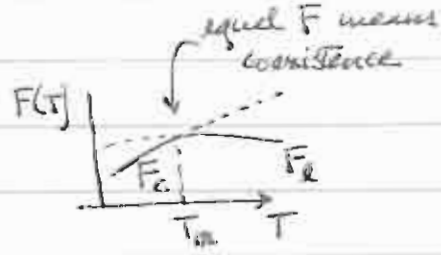
Prob 2

(a) $P \sim e^{-\int_E^{E'} \frac{\Sigma_s''}{\Sigma_t''}\frac{dE''}{\xi E''}}$ MCNP - start neutron at energy E', track until neut. crosses E or is absorbed whichever is first
tally ratio # crossing / # started

(b) $\phi(\tilde{R} = R + 2D) = 0$ MCNP -- simulate reactor, run flux tally plot flux & linearly extrapolate to zero to determine $\tilde{R}$

Prob 3

(a) $F = E - TS$, entropy S is difficult to calc.
thermodyn def of melting $F_{crystal}(T_m) = F_{liq}(T_m)$



knowing F is not enough to discuss how melting occurs

(b) MC: system evolves by particles making random displacements sequentially, moves accepted or rejected according to energy criterion, system can go 'uphill'

MD: evolves by particle displacements in time collectively, moves made according to interatomic forces (solving Newton's eq. of motion)

study melting —

MC can evaluate F, can calc. eq. structure of crystal or liq., therefore determine T_m

MD can look at kinetics directly, such as the effect of a surface or defects, can do what MC can do (maybe not so computationally efficient), plus MD can give dynamical behavior at short times

equilibrium (time indep) properties calc. by MC and MD should be the <u>same</u>

dynamical (time-dep) properties should be <u>different</u>

<u>Prob 4</u>

(a) Born approx. $f(\theta) \sim \int d^3r\, e^{i\underline{K}\cdot\underline{r}} V(r)$

Fermi pseudopotential (N particles) $V(r, R_1, \ldots, R_N) \sim \sum_{\ell=1}^{N} a_\ell \delta(\underline{r} - \underline{R}_\ell)$

integral eq. formulation

$$\psi \sim e^{ik\cdot r} + f(\theta)\frac{e^{ikr}}{r} \rightarrow f_{n_c n}(\theta) = -\sum_{\ell=1}^{N} a_\ell \langle n | e^{i\underline{K}\cdot\underline{R}_\ell} | n_c \rangle$$

(b) $$\bar{I} \sim \sum_{\ell\ell'} \overline{a_\ell a_{\ell'}}\, \psi^*(\ell)\psi(\ell')$$

$\ell = \ell'$ $\quad \overline{a_\ell a_\ell} = \overline{a^2}$

$\ell \neq \ell'$ $\quad \overline{a_\ell a_{\ell'}} = \bar{a}_\ell \bar{a}_{\ell'} = \bar{a}^2$

$$\underbrace{(\overline{a^2} - \bar{a}^2)}_{a^2_{inc}} \delta_{\ell\ell'} + \underbrace{\bar{a}^2}_{a^2_{coh}}$$

$$\tilde{I} \sim a^2_{inc} \sum_\ell |\psi(\ell)|^2 + a^2_{coh} \sum_{\ell\ell'} \psi^*(\ell)\psi(\ell')$$

self scattering (individual particle) — collective scattering (self + interference)