Outline of tb.c Programming

Required Utility Functions: `https://aiichironakano.github.io/phys516/src/TB/`

1. tb_util_angstrom.c or tb_util_au.c: Copy contents of either one into your header and program files (name them tb.h and tb.c, respectively)
2. eigen.c: To be compiled together with your tb.c

Additional Utility Function: `https://aiichironakano.github.io/phys516/src/MD/`

1. *SignR*() function in md.h to implement periodic boundary condition (PBC)

Algorithm

```
Read InitUcell[3]        // How many times to repeat the diamond unit cell (in tb_util.c)
InitConf() → $nAtom \leftarrow 8\prod_{a=0}^{2} IntiUcell[a]$
             $r[0{:}nAtom-1][0{:}2]$        // $r[i][0|1|2] = r_{i,x|y|z}$, where $\vec{r}_i = (r_{i,x}, r_{i,y}, r_{i,z})$

int n4 = 4×nAtom        // Vector length
double** h = dmatrix(1,n4,1,n4)        // Allocate memory and allow the use of h[1:n4][1:n4]
double* d = dvector(1,n4)              // Allocate d[1:n4]
double* e = dvector(1,n4)              // Allocate e[1:n4]; dmatrix and dvector() defined in eigen.c[*]

// Set up h[1:n4][1:n4]
for $1 \le i \le n4$
    for $1 \le j \le n4$
        $h[i][j] \leftarrow 0$
for $0 \le i < nAtom$
    // Fill diagonal (intra-atom) block
    $\begin{cases} h[4i+1][4i+1] \leftarrow E_s \\ h[4i+k][4i+k] \leftarrow E_p (k = 2,3,4) \end{cases}$
    for $i+1 \le j < nAtom$
        $\vec{r}_{ij} \leftarrow \vec{r}_i - \vec{r}_j = (r_{ij,x}, r_{ij,y}, r_{ij,z})$
        // Pick the minimum image (cf. ComputeAccel() in md.c)
        $r_{ij,a} = r_{ij,a} - SignR\left(\frac{L_a}{2}, r_{ij,a} - \frac{L_a}{2}\right) - SignR\left(\frac{L_a}{2}, r_{ij,a} + \frac{L_a}{2}\right)\ (a = 0,1,2)$
        Here, $\frac{L_a}{2} = \frac{1}{2} \times \underbrace{LCNS}_{\text{lattice constant}} \times InitUcell[a] \rightarrow RegionH[3]$
        $\hat{d} \leftarrow \vec{r}_{ij} / \underbrace{|\vec{r}_{ij}|}_{r} = (d_x, d_y, d_z)$  // Unit-length bond-direction vector
        Fill off-diagonal block, $h[4i+k][4j+l]\ (k,l = 1,2,3,4)$
        Symmetric copy: $h[4j+l][4i+k] = h[4i+k][4j+l]\ (k,l = 1,2,3,4)$
```

[*] Don't forget to prototype *dmatrix*() and *dvector*(), which are defined in eigen.c, in your header file, tb.h.

```
double **dmatrix(int, int, int, int);
double *dvector(int, int);
```

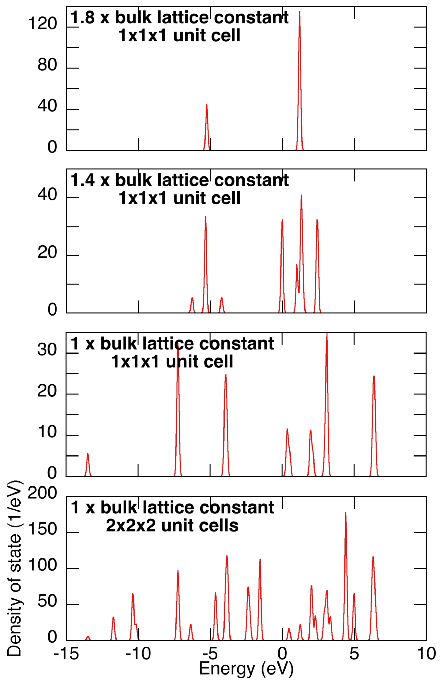
```
// Diagonalize the Hamiltonian matrix[†]
tred2(h,n4,d,e)
tqli(d,e,n4,h)    // Now d[1:n4] hold the eigenvalues (not sorted)

// Sort the eigenvalues in ascending order[‡]
for $1 \le i < n4$
    for $i + 1 \le j \le n4$
        if $d[i] > d[j]$
            // Swap the elements
            $dummy \leftarrow d[i]$
            $d[i] \leftarrow d[j]$
            $d[j] \leftarrow dummy$

// Plot the electronic density of states (DOS)
$\varepsilon_{\min}$ = -15.0 [eV]     // Minimum and maximum energies to plot DOS
$\varepsilon_{\max}$ = 10.0 [eV]
$\sigma$ = 0.1 [eV]             // Smear each eigenvalue as a Gaussian function
for $0 \le i < Nbin$        // Use the number of energy bins Nbin = 500
    $\varepsilon_i \leftarrow \varepsilon_{min} + i\frac{\varepsilon_{\max}-\varepsilon_{min}}{Nbin}$
    $D(\varepsilon_i) \leftarrow \sum_{v=1}^{n4}\frac{1}{\sqrt{\pi}\sigma}\exp\left[-\frac{(\varepsilon_i-\varepsilon_v)^2}{\sigma^2}\right]$
    Plot $\varepsilon_i$ vs. $D(\varepsilon_i)$
```

Compile and Run

Compile: cc –o tb tb.c eigen.c -lm

Run: *LCNS* = 5.43 Å (or 10.2622 a.u.) × 1.0 | 1.4 | 1.8; *InitUcell*[3] = (1, 1, 1), 8 atoms

LCNS = 5.43 Å (or 10.2622 a.u.); *InitUcell*[3] = (2, 2, 2), 64 atoms



[†] Don't forget to prototype *tred2*() and *tqli*(), which are defined in eigen.c, in your header file, tb.h.
    void tred2(double **, int, double *, double *);
    void tqli(double *, double *, int, double **);

[‡] Upon return from *tqli*(), *h*[1:*n4*][*i*] and *h*[1:*n4*][*j*] store *i*-th and *j*-th eivenvectors; these columns need be swapped as well, if we need to use them (not necessary for the homework).