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clear;
close all;

c=2.998e10;%cm/s
hbar=6.582e-16; %in eV*sec
m=5.11e5/c^2; %in eV/c^2

dx=0.7e-8; %1 Ang, in cm
dy=dx;
dz=dx;

tx=-hbar^2/(2*m*dx^2);
ty=-hbar^2/(2*m*dy^2);
tz=-hbar^2/(2*m*dz^2);

Nx=18;
Ny=Nx;
Nz=Nx;

Hx=-2*(tx+ty+tz)*eye(Nx)+diag(tx*ones(Nx-1,1),1)+diag(tx*ones(Nx-1,1),-1);
Hy=ty*eye(Nx);
Hz=tz*eye(Nx*Ny);

Hxy=kron(eye(Ny),Hx)+kron(diag(ones(Ny-1,1),1),Hy)+kron(diag(ones(Ny-1,1),-1),Hy);
H=kron(eye(Nz),Hxy)+kron(diag(ones(Nz-1,1),1),Hz)+kron(diag(ones(Nz-1,1),-1),Hz);

%add infinite spherical potential; radius is Nx/2*dx
V=zeros(Nx*Ny*Nz,1);
for ii=1:Nx
    for jj=1:Ny
        for kk=1:Nz
            if ((ii-(Nx+1)/2)^2*dx^2+...
                (jj-(Ny+1)/2)^2*dy^2+...
                (kk-(Nz+1)/2)^2*dz^2)>=(Nx/2*dx)^2
                V((kk-1)*(Nx*Ny)+(jj-1)*Nx+ii)=1000;
            end
        end
    end
end

H=sparse(H+diag(V));

NUMEs=20;
[v,d]=eigs(H,NUMEs,'SM');%use MATLAB eigs()

E=diag(d);

figure(99)

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plot(sort(E),'*');
xlabel('eigenvalue');
ylabel('energy [eV]');

v=fliplr(v);
vsv=conj(v).*v;

for ii=1:10
    psistarpsi=reshape(vsv(:,ii),Nx, Ny, Nz);
    eval(['figure(' int2str(ii) ')']);
    isosurface(psistarpsi,0.0005);
    xlabel('X'); ylabel('Y')
end

figure(100);
V3D=reshape(V,Nx, Ny, Nz);
isosurface(V3D,1);
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