PHYS 513 Midterm - Neema Badihian

1. $Fe_4 S_4$

Fe	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$	19	4	76	152
S	$1s^2 2s^2 2p^6 3s^2 3p^4$	9	4	36	72

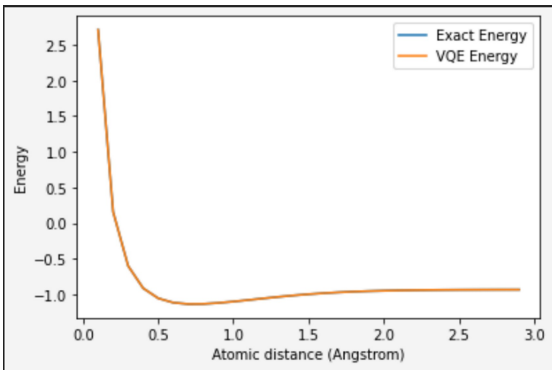
144 + 72 = 224

$\log_2(224) = 7.8074$

Approximately 8 qubits are needed.

2. B.

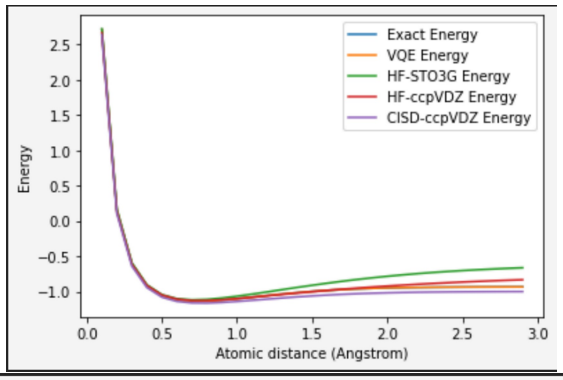
1)



Distances	Exact Energy	VQE Energy
0.1	[2.70996077]	(2.709960770869062+0j)
0.2	[0.15748213]	(0.15748213480149253+0j)
0.30000000000000004	[-0.60180371]	(-0.6018037107600802+0j)
0.4	[-0.9141497]	(-0.9141497046154452+0j)
0.5	[-1.05515979]	(-1.0551597944480278+0j)
0.6	[-1.11628601]	(-1.1162860068303306+0j)
0.7000000000000001	[-1.13618945]	(-1.1361894540110444+0j)
0.8	[-1.13414767]	(-1.1341476666206636+0j)
0.9	[-1.12056028]	(-1.1205601297735766+0j)
1.0	[-1.10115033]	(-1.101150318805789+0j)
1.1	[-1.07919294]	(-1.0791929449548878+0j)
1.2000000000000002	[-1.05674075]	(-1.056740744935825+0j)
1.3000000000000003	[-1.03518627]	(-1.035186263803602+0j)
1.4000000000000001	[-1.01546825]	(-1.0154682470682 62+0j)
1.5000000000000002	[-0.99814935]	(-0.9981493525206409+0j)
1.6	[-0.98347273]	(-0.9834727288653822+0j)
1.7000000000000002	[-0.97142669]	(-0.971426688452492+0j)
1.8000000000000003	[-0.96181695]	(-0.9618166583890703+0j)
1.9000000000000001	[-0.95433885]	(-0.9543388539973632+0j)
2.0	[-0.94864111]	(-0.9486411120438953+0j)
2.1	[-0.94437468]	(-0.9443746796799168+0j)
2.2	[-0.94122403]	(-0.9412240270584951+0j)
2.3000000000000003	[-0.93892239]	(-0.9389223672352991+0j)
2.4000000000000004	[-0.93725495]	(-0.9372549143156487+0j)
2.5000000000000004	[-0.93605492]	(-0.9360548559137458+0j)
2.6	[-0.93519603]	(-0.9351959404476122+0j)
2.7	[-0.93458442]	(-0.9345843025952387+0j)
2.8000000000000003	[-0.9341511]	(-0.9341509654869509+0j)
2.9000000000000004	[-0.93384575]	(-0.9338456108396836+0j)

2)

```
for dist in distances:
    mol_sto3g = pyscf.M(
        atom = "H .0 .0 .0; H .0 .0 " + str(dist),
        spin = 0,
        charge = 0,
        basis = "sto3g")
    mol_ccpvdz = pyscf.M(
        atom = "H .0 .0 .0; H .0 .0 " + str(dist),
        spin = 0,
        charge = 0,
        basis = "ccpvdz")
    mf_sto3g = mol_sto3g.HF().run()
    mf_ccpvdz = mol_ccpvdz.HF().run()
    mycc_ccpvdz = mf_ccpvdz.CISD().run()
    hf_sto3g_energies.append(mf_sto3g.e_tot)
    hf_ccpvdz_energies.append(mf_ccpvdz.e_tot)
    cisd_ccpvdz_energies.append(mycc_ccpvdz.e_tot)
print("Alternate basis sets have been calculated")
```



Distances	Exact Energy	VQE Energy	HF-STO3G Energy	HF-ccpVDZ Energy	CISD-ccpVDZ Energy
0.1	[2.70996077]	(2.709960770869062+0j)	2.7158873932927525	2.660900474741531	2.63724894546576
0.2	[0.15748213]	(0.15748213480149253+0j)	0.16417501206169538	0.13222212152276125	0.10710273165855676
0.30000000000000004	[-0.60180371]	(-0.6018037107600802+0j)	-0.5938277585357274	-0.6118500477798807	-0.6387775195330653
0.4	[-0.9141497]	(-0.9141497046154452+0j)	-0.9043613941635398	-0.9143486914708849	-0.9431336135048608
0.5	[-1.05515979]	(-1.0551597944480278+0j)	-1.042996274540095	-1.0488005562126916	-1.079370050878104
0.6	[-1.11628601]	(-1.1162860068303306+0j)	-1.1011282422677018	-1.1068924751448512	-1.1391732932872087
0.7000000000000001	[-1.13618945]	(-1.1361894540110444+0j)	-1.117349034990279	-1.1269246923009137	-1.1609046824774614
0.8	[-1.13414767]	(-1.1341476666206636+0j)	-1.1108503974765953	-1.1270007208841992	-1.1627507630215572
0.9	[-1.12056028]	(-1.1205601297735766+0j)	-1.091914041020057	-1.116391300444487	-1.154081706117267
1.0	[-1.10115033]	(-1.101150318805789+0j)	-1.0661086493179366	-1.1001537648784097	-1.1400734808675144
1.1	[-1.07919294]	(-1.0791929449548878+0j)	-1.03653887502918	-1.0811707843775875	-1.1237352366097357
1.2000000000000002	[-1.05674075]	(-1.056740744935825+0j)	-1.00510670656849	-1.0611119978574888	-1.1068551925545187
1.3000000000000003	[-1.03518627]	(-1.0351862638033602+0j)	-0.973110615777578	-1.0409387385167304	-1.0904938660285677
1.4000000000000001	[-1.01546825]	(-1.015468247068262+0j)	-0.9414806547077985	-1.0211968374074127	-1.0752705377413962
1.5000000000000002	[-0.99814935]	(-0.9981493525206409+0j)	-0.9108735545943862	-1.0021927454865378	-1.0615349496305058
1.6	[-0.98347273]	(-0.9834727288653822+0j)	-0.8817324499460566	-0.9840967891557333	-1.0494644468980903
1.7000000000000002	[-0.97142669]	(-0.971426688452492+0j)	-0.8543376269512921	-0.9669994539478846	-1.0391133471436018
1.8000000000000003	[-0.96181695]	(-0.9618166583890703+0j)	-0.8288481479269773	-0.9509393584651203	-1.0304388190697193
1.9000000000000001	[-0.95433885]	(-0.9543388539973632+0j)	-0.8053328448932773	-0.9359176828185161	-1.023322284361851
2.0	[-0.94864111]	(-0.9486411120438953+0j)	-0.783792654277353	-0.9219085941148848	-1.017594114044795
2.1	[-0.94437468]	(-0.9443746796799168+0j)	-0.7641776516167973	-0.9088689039402806	-1.0130594576969008
2.2	[-0.94122403]	(-0.9412240270584951+0j)	-0.7464013499911591	-0.8967463575743762	-1.009520288334115
2.3000000000000003	[-0.93892239]	(-0.9389223672352991+0j)	-0.7303533213548868	-0.8854855184790436	-1.0067909397832084
2.4000000000000004	[-0.93725495]	(-0.9372549143156487+0j)	-0.7159100604538067	-0.8750312001701331	-1.0047070596402068
2.5000000000000004	[-0.93605492]	(-0.9360548559137458+0j)	-0.7029435997235265	-0.865330120145507	-1.003129251223641
2.6	[-0.93519603]	(-0.9351959404476122+0j)	-0.6913275611973779	-0.8563315618647145	-1.001943029411738
2.7	[-0.93458442]	(-0.9345843025952387+0j)	-0.6809407606225886	-0.847987609235799	-1.0010566028498147
2.8000000000000003	[-0.9341511]	(-0.9341509654869509+0j)	-0.671668859751728	-0.8402532413836741	-1.0003976766669358
2.9000000000000004	[-0.93384575]	(-0.9338456108396836+0j)	-0.6634047415990408	-0.8330863749345013	-0.999910074988683

The minimum-energy distance for VQE is the same for the Exact Energy and the HF-STO3G Energy, 0.7. The HF-ccpVDZ and CISD-ccpVDZ minimum-energy distance is slightly higher at 0.8. As for minimum energy, VQE appears to have the lowest energy compared to the other methods when the distance is 0.7 with -1.13618945. VQE has the same minimum-energy distance and minimum energy as the exact energy. HF appears to be less optimal compared to the CISD as HF's trajectory, for both STO3G and ccpVDZ, seems to increase while CISD stays practically parallel to VQE and Exact Energy.