QM1 Exam- Problem 11, Partial solution

Omri Golan

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golanomri@gmail.com

Problem 11: Consider the following Hamiltonian

$$H=\int\psi^{\dagger}(x)\left(-\frac{\hbar^{2}}{2m}\partial_{x}^{2}\right)\psi(x)\,\mathrm{d}x+\int\left(\psi^{\dagger}(x)+\psi(x)\right)V(x-y)\,\mu_{3}(y)\,\mathrm{d}x\mathrm{d}y+\int\mu_{1}(y)\,\mathrm{d}y \tag{1}$$

$$\mu_{j}(y)=\frac{1}{2}\sum_{\alpha,\beta=\pm1}\xi_{\alpha}^{\dagger}(y)\,\sigma_{j}^{\alpha\beta}\xi_{\beta}(y)=\frac{1}{2}\xi_{\alpha}^{\dagger}(y)\,\sigma_{j}^{\alpha\beta}\xi_{\beta}(y) \tag{2}$$

where $\psi(x)$ and $\psi^{\dagger}(x)$ are boson operators, $\xi_{\alpha}^{\dagger}(y)$ and $\xi_{\alpha}(y)$ are fermion operators, σ_j are the Pauli matrices and $V(x-y)=\lambda\delta(x-y)$.

1. Use variational approximation with factorized wave function

$$|\Psi\rangle=|bosons\rangle\,|fermions\rangle \tag{3}$$

for a ground state of H with one fermion and arbitrary number of bosons. (Hint: a) use your experience with a similarly looking home- work problem b) good notation will take you far c) you may find it a bit easier to do some of the calculations in momentum representation) What is the meaning of the infinite energy term which you obtain in your solution?

2. Repeat 1. for several fermions.

Reminder of problem 3 from problem set 5

Consider the following Hamiltonian

$$H=\int\psi^{\dagger}(x)\left(-\frac{\hbar^{2}}{2m}\partial_{x}^{2}\right)\psi(x)\,\mathrm{d}x+\int\left(\psi^{\dagger}(x)+\psi(x)\right)V(x-y)\,\mu(y)\,\mathrm{d}x\mathrm{d}y=K+V \tag{4}$$

where $\psi(x)$ and $\psi^{\dagger}(x)$ are boson operators,

$$\mu(y)=\frac{1}{2}\sum_{\alpha,\beta=\pm1}\xi_{\alpha}^{\dagger}(y)\,\sigma_{\alpha\beta}^{z}\xi_{\beta}(y) \tag{5}$$

$\xi_{\alpha}^{\dagger}(y)$ and $\xi_{\alpha}(y)$ are fermion operators, σ^z is the Pauli matrix and $V(x-y)=\lambda\delta(x-y)$.

Find eigenstates and eigenvalues of H with an arbitrary number of fermions and arbitrary number of bosons. (Hint: you may find it a bit easier to do some of the calculations in momentum representation) What is the meaning of the infinite energy term which you obtain in your solution?

Solution: Useful commutators:

$$\left[\psi\left(z\right),\prod_{i=1}^{N}\psi^{\dagger}\left(x_{i}\right)\right]=\left[\psi\left(z\right),\psi^{\dagger}\left(x_{N}\right)\prod_{i=1}^{N-1}\psi^{\dagger}\left(x_{i}\right)\right]= \tag{6}$$

$$=\psi^{\dagger}\left(x_{N_f}\right)\left[\psi\left(z\right),\prod_{i=1}^{N-1}\psi^{\dagger}\left(x_{i}\right)\right]+\left[\psi\left(z\right),\psi^{\dagger}\left(x_{N}\right)\right]\prod_{i=1}^{N-1}\psi^{\dagger}\left(x_{i}\right)=$$

$$=\psi^{\dagger}\left(x_{N_f}\right)\left[\psi\left(z\right),\prod_{i=1}^{N-1}\psi^{\dagger}\left(x_{i}\right)\right]+\delta\left(z-x_{N}\right)\prod_{i=1}^{N_b-1}\psi^{\dagger}\left(x_{i}\right)=$$

$$=\cdots=\sum_{i=1}^{N}\delta\left(z-x_{i}\right)\prod_{i\neq j=1}^{N}\psi^{\dagger}\left(x_{j}\right)$$

$$\left\{\xi_{a}\left(z\right),\prod_{j=1}^{N}\xi_{\alpha_j}^{\dagger}\left(y_{j}\right)\right\}=\sum_{k=1}^{N}\left(-1\right)^{N-k}\delta_{a,\alpha_k}\delta\left(z-y_{k}\right)\prod_{k\neq j=1}^{N}\xi_{\alpha_j}^{\dagger}\left(y_{j}\right) \tag{7}$$

$$\Rightarrow\quad \xi_{a}\left(z\right)\prod_{j=1}^{N}\xi_{\alpha_j}^{\dagger}\left(y_{j}\right)\left|0\right\rangle=\sum_{k=1}^{N}\left(-1\right)^{N-k}\delta_{a,\alpha_k}\delta\left(z-y_{k}\right)\prod_{k\neq j=1}^{N}\xi_{\alpha_j}^{\dagger}\left(y_{j}\right)\left|0\right\rangle \tag{8}$$

$$\Rightarrow\quad \xi_{a}^{\dagger}\left(z\right)\xi_{a}\left(z\right)\prod_{j=1}^{N}\xi_{\alpha_j}^{\dagger}\left(y_{j}\right)\left|0\right\rangle=\sum_{k=1}^{N}\delta_{a,\alpha_k}\delta\left(z-y_{k}\right)\prod_{j=1}^{N}\xi_{\alpha_j}^{\dagger}\left(y_{j}\right)\left|0\right\rangle \tag{9}$$

Inserting the Fourier transform $\psi\left(x\right)=\int\frac{\mathrm{d}k}{2\pi}a_{k}e^{ikx}$ into the Hamiltonian gives

$$H=\int\psi^{\dagger}\left(x\right)\left(-\frac{\hbar^{2}}{2m}\partial_{x}^{2}\right)\psi\left(x\right)\mathrm{d}x+\int\left(\psi^{\dagger}\left(x\right)+\psi\left(x\right)\right)V\left(x-y\right)\mu\left(y\right)\mathrm{d}x\mathrm{d}y=K+V \tag{10}$$

$$K=\int\psi^{\dagger}\left(x\right)\left(-\frac{\hbar^{2}}{2m}\partial_{x}^{2}\right)\psi\left(x\right)\mathrm{d}x=\int\frac{\mathrm{d}k}{2\pi}\frac{\hbar^{2}k^{2}}{2m}a_{k}^{\dagger}a_{k}; \tag{11}$$

$$V=\lambda\int\left(\psi^{\dagger}\left(x\right)+\psi\left(x\right)\right)\mu\left(x\right)\mathrm{d}x=\lambda\int\frac{\mathrm{d}k}{2\pi}\mathrm{d}x\left(a_{k}^{\dagger}e^{-ikx}+a_{k}e^{ikx}\right)\mu\left(x\right)\mathrm{d}x; \tag{12}$$

Note that

$$\left[a_{k},a_{q}^{\dagger}\right]=\left[\int\mathrm{d}x\psi\left(x\right)e^{-ikx},\int\mathrm{d}y\psi^{\dagger}\left(y\right)e^{iqy}\right]=\int\mathrm{d}x\mathrm{d}y\delta\left(x-y\right)e^{-ikx}e^{iqy}= \tag{13}$$

$$=\int\mathrm{d}xe^{-ikx}e^{iqx}=2\pi\delta\left(k-q\right) \tag{14}$$

The general state with N_f fermions at positions $y_1,\cdots,y_{N_f}$ can be written as

$$\left|F\right\rangle=J\left[a^{\dagger}\right]\prod_{j=1}^{N_f}\xi_{\alpha_j}^{\dagger}\left(y_{j}\right)\left|0\right\rangle \tag{15}$$

where $J\left[a^\dagger\right]$ is some functional depending on $\left\{a_k^\dagger\right\}_k$. Acting with H on $|F\rangle$ gives

$$K|F\rangle=\int \mathrm{d}k\frac{\hbar^2k^2}{2m}a_k^\dagger a_k J\left[a^\dagger\right]\prod_{j=1}^{N_f}\xi_{\alpha_j}^\dagger\left(y_j\right)|0\rangle= \tag{16}$$

$$\prod_{j=1}^{N_f}\xi_{\alpha_j}^\dagger\left(y_j\right)\int \mathrm{d}k\frac{\hbar^2k^2}{2m}a_k^\dagger a_k J\left[a^\dagger\right]|0\rangle;$$

$$V|F\rangle=\lambda\int\frac{\mathrm{d}k}{2\pi}\mathrm{d}x\left(a_k^\dagger e^{-ikx}+a_k e^{ikx}\right)\mu\left(x\right)J\left[a^\dagger\right]\prod_{j=1}^{N_f}\xi_{\alpha_j}^\dagger\left(y_j\right)|0\rangle= \tag{17}$$

$$\lambda\int\frac{\mathrm{d}k}{2\pi}\mathrm{d}x\left(a_k^\dagger e^{-ikx}+a_k e^{ikx}\right)\frac{1}{2}\xi_a^\dagger\left(x\right)\sigma_{ab}^z\xi_b\left(x\right)J\left[a^\dagger\right]\prod_{j=1}^{N_f}\xi_{\alpha_j}^\dagger\left(y_j\right)|0\rangle=$$

$$\lambda\int\frac{\mathrm{d}k}{2\pi}\mathrm{d}x\left(a_k^\dagger e^{-ikx}+a_k e^{ikx}\right)J\left[a^\dagger\right]\frac{1}{2}\sum_{a=\pm1}a\xi_a^\dagger\left(x\right)\xi_a\left(x\right)\prod_{j=1}^{N_f}\xi_{\alpha_j}^\dagger\left(y_j\right)|0\rangle=$$

$$\lambda\int\frac{\mathrm{d}k}{2\pi}\mathrm{d}x\left(a_k^\dagger e^{-ikx}+a_k e^{ikx}\right)J\left[a^\dagger\right]\frac{1}{2}\sum_{a=\pm1}a\sum_{m=1}^{N_f}\delta_{a,\alpha_m}\delta\left(x-y_m\right)\prod_{j=1}^{N_f}\xi_{\alpha_j}^\dagger\left(y_j\right)|0\rangle=$$

$$\prod_{j=1}^{N}\xi_{\alpha_j}^\dagger\left(y_j\right)\frac{\lambda}{2}\sum_{m=1}^{N_f}\int\frac{\mathrm{d}k}{2\pi}\left(a_k^\dagger e^{-iky_m}+a_k e^{iky_m}\right)\alpha_m J\left[a^\dagger\right]|0\rangle;$$

Taking anti commutators with the ξs we see that the eigenvalue equation is equivalent to

$$\int\frac{\mathrm{d}k}{2\pi}\left[\frac{\hbar^2k^2}{2m}a_k^\dagger a_k+\frac{\lambda}{2}\sum_{k=1}^{N_f}\left(a_k^\dagger e^{-iky_m}+a_k e^{iky_m}\right)\alpha_m\right]J\left[a^\dagger\right]|0\rangle=EJ\left[a^\dagger\right]|0\rangle \tag{18}$$

In the case of a single fermion this reduces to

$$\int\frac{\mathrm{d}k}{2\pi}\left[\frac{\hbar^2k^2}{2m}a_k^\dagger a_k+\frac{\lambda}{2}\alpha\left(a_k^\dagger e^{-iky}+a_k e^{iky}\right)\right]J\left[a^\dagger\right]|0\rangle=EJ\left[a^\dagger\right]|0\rangle \tag{19}$$

In terms of the operator $b_k=a_k+\alpha\frac{m\lambda}{\hbar^2k^2}e^{-iky}$,

$$EJ\left[a^\dagger\right]|0\rangle=\int\frac{\mathrm{d}k}{2\pi}\frac{\hbar^2k^2}{2m}\left[a_k^\dagger a_k+\alpha\frac{m\lambda}{\hbar^2k^2}\left(a_k^\dagger e^{-iky}+a_k e^{iky}\right)\right]J\left[a^\dagger\right]|0\rangle= \tag{20}$$

$$\int\frac{\mathrm{d}k}{2\pi}\frac{\hbar^2k^2}{2m}\left[b_k^\dagger b_k-\left(\frac{m\lambda}{\hbar^2k^2}\right)^2\right]J\left[a^\dagger\right]|0\rangle=\int\frac{\mathrm{d}k}{2\pi}\left[\frac{\hbar^2k^2}{2m}b_k^\dagger b_k-\frac{m\lambda^2}{2\hbar^2k^2}\right]J\left[a^\dagger\right]|0\rangle \tag{21}$$

$$\Rightarrow\quad\int\frac{\mathrm{d}k}{2\pi}\frac{\hbar^2k^2}{2m}b_k^\dagger b_k J\left[a^\dagger\right]|0\rangle=\left(E+\int\frac{\mathrm{d}k}{2\pi}\frac{m\lambda^2}{2\hbar^2k^2}\right)J\left[a^\dagger\right]|0\rangle \tag{22}$$

where we have used

$$b_k^\dagger b_k=\left(a_k^\dagger+\alpha\frac{m\lambda}{\hbar^2k^2}e^{iky}\right)\left(a_k+\alpha\frac{m\lambda}{\hbar^2k^2}e^{-iky}\right)= \tag{23}$$

$$=a_k^\dagger a_k+\alpha\frac{m\lambda}{\hbar^2k^2}\left(a_k^\dagger e^{-iky}+a_k e^{iky}\right)+\left(\frac{m\lambda}{\hbar^2k^2}\right)^2 \tag{24}$$

Now, note that the b_ks are also boson annihilation operators, since

$$\left[b_k,b_q^\dagger\right]=2\pi\delta\left(k-q\right),\ \left[b_k^\dagger,b_q^\dagger\right]=\left[b_k,b_q\right]=0 \tag{25}$$

Therefore the states they create, $\prod_{i=1}^{N} b_{k_i}^{\dagger}|0\rangle$, will be orthogonal. These states also span the Fock space because the states $\prod_{i=1}^{N} a_{k_i}^{\dagger}|0\rangle$ span the Fock space and $\left(a_k^{\dagger}\right)^n = \left(b_k^{\dagger} - \alpha\frac{m\lambda}{\hbar^2 k^2}e^{iky}\right)^n$ is a sum of powers of b_k. Hence the bs create the entire Fock space, and passing from the as to the bs is equivalent to a change of basis (but not to a single particle basis, since we mix the single particle states with the vacuum). From (22) we see that the states $\prod_{i=1}^{N} b_{k_i}^{\dagger}|0\rangle$ are eigenstates of H,

$$H\prod_{i=1}^{N} b_{k_i}^{\dagger}|0\rangle = \int\frac{\mathrm{d}k}{2\pi}\left[\frac{\hbar^2k^2}{2m}b_k^{\dagger}b_k - \frac{m\lambda^2}{2\hbar^2k^2}\right]\prod_{i=1}^{N} b_{k_i}^{\dagger}|0\rangle = \tag{26}$$

$$\int\frac{\mathrm{d}k}{2\pi}\left[2\pi\frac{\hbar^2k^2}{2m}\sum_{i=1}^{N}\delta\left(k-k_i\right) - \frac{m\lambda^2}{2\hbar^2k^2}\right]\prod_{i=1}^{N} b_{k_i}^{\dagger}|0\rangle = \tag{27}$$

$$\left(\sum_{i=1}^{N}\frac{\hbar^2k_i^2}{2m} - \int\frac{\mathrm{d}k}{2\pi}\frac{m\lambda^2}{2\hbar^2k^2}\right)\prod_{i=1}^{N} b_{k_i}^{\dagger}|0\rangle \tag{28}$$

$$\Rightarrow\quad E = \sum_{i=1}^{N}\frac{\hbar^2k_i^2}{2m} - \int\frac{\mathrm{d}k}{2\pi}\frac{m\lambda^2}{2\hbar^2k^2} \tag{29}$$

The energies include the term $\int\frac{\mathrm{d}k}{2\pi}\frac{m\lambda^2}{2\hbar^2k^2}$. In one dimension $\int_{-\infty}^{\infty}\frac{\mathrm{d}k}{2\pi}\frac{m\lambda^2}{2\hbar^2k^2} = +\infty$ because of the divergence at $k=0$. At higher dimensions is will diverges due to the contribution from $|k| = \infty$ (in two dimensions it diverges on both ends). Both these problems are solved if we work in a finite box and on a lattice. These will generate lower and upper cutoffs on the wave number $|k|$. I don't have anything interesting to say about the source of this divergence...

To summarize, the one fermion eigenstates and energies of H are

$$|F\rangle = \xi_{\alpha}(y)\,J\left[a^{\dagger}\right]|0\rangle = \xi_{\alpha}(y)\prod_{i=1}^{N} b_{k_i}^{\dagger}|0\rangle = \xi_{\alpha}(y)\prod_{i=1}^{N}\left(a_{k_i}^{\dagger} + \alpha\frac{m\lambda}{\hbar^2k_i^2}e^{-ik_iy}\right)|0\rangle \tag{30}$$

$$E\left(\{k_i\}_{i=1}^{N}\right) = \sum_{i=1}^{N}\frac{\hbar^2k_i^2}{2m} - \int\frac{\mathrm{d}k}{2\pi}\frac{m\lambda^2}{2\hbar^2k^2} \tag{31}$$

Note that the energies do not depend on the fermionic numbers y, α, but the states do depend on them.

Now for the case of N_f fermions. We already obtained

$$\int\frac{\mathrm{d}k}{2\pi}\left[\frac{\hbar^2k^2}{2m}a_k^{\dagger}a_k + \frac{\lambda}{2}\sum_{k=1}^{N_f}\left(a_k^{\dagger}e^{-iky_m} + a_ke^{iky_m}\right)\alpha_m\right]J\left[a^{\dagger}\right]|0\rangle = EJ\left[a^{\dagger}\right]|0\rangle \tag{32}$$

We define

$$b_k = a_k + \sum_{m=1}^{N_f}\alpha_m\frac{m\lambda}{\hbar^2k^2}e^{-iky_m} \tag{33}$$

$$b_k^{\dagger}b_k = \left(a_k^{\dagger} + \sum_{m=1}^{N_f}\alpha_m\frac{m\lambda}{\hbar^2k^2}e^{iky_m}\right)\left(a_k + \sum_{m=1}^{N_f}\alpha_m\frac{m\lambda}{\hbar^2k^2}e^{-iky_m}\right) = \tag{34}$$

$$= a_k^{\dagger}a_k + \sum_{m=1}^{N_f}\alpha_m\frac{m\lambda}{\hbar^2k^2}\left(a_k^{\dagger}e^{-iky_m} + a_ke^{iky_m}\right) + \left(\frac{m\lambda}{\hbar^2k^2}\right)^2\sum_{n,m=1}^{N_f}\alpha_n\alpha_me^{ik(y_m-y_n)} \tag{35}$$

in terms of which equation (32) takes the simple form

$$\int\frac{\mathrm{d}k}{2\pi}\left[\frac{\hbar^2k^2}{2m}b_k^{\dagger}b_k - \int\frac{\mathrm{d}k}{2\pi}\frac{m\lambda^2}{2\hbar^2k^2}\sum_{n,m=1}^{N_f}\alpha_n\alpha_me^{ik(y_m-y_n)}\right]J\left[a^{\dagger}\right]|0\rangle = EJ\left[a^{\dagger}\right]|0\rangle \tag{36}$$

The states and energies are therefore

$$|F\rangle=\xi_\alpha\left(y\right)J\left[a^\dagger\right]|0\rangle=\xi_\alpha\left(y\right)\prod_{i=1}^{N_b}b_{k_i}^\dagger|0\rangle=\prod_{j=1}^{N_f}\xi_{\alpha_j}\left(y_j\right)\prod_{i=1}^{N_b}\left(a_{k_i}^\dagger+\sum_{j=1}^{N_f}\alpha_j\frac{m\lambda}{\hbar^2k_i^2}e^{-ik_iy_j}\right)|0\rangle \tag{37}$$

$$E\left(\left\{y_j\right\}_{j=1}^{N_f},\left\{\alpha_j\right\}_{j=1}^{N_f},\left\{k_i\right\}_{i=1}^{N}\right)=\sum_{i=1}^{N_b}\frac{\hbar^2k_i^2}{2m}-\int\frac{\mathrm{d}k}{2\pi}\frac{m\lambda^2}{2\hbar^2k^2}\sum_{n,m=1}^{N_f}\alpha_n\alpha_me^{ik(y_m-y_n)} \tag{38}$$

Note that now the energies depend on all fermionic numbers, and if two fermions are in the same position but have opposite spins, their effects on both the bosonic states and the energies cancel. We have the same infinities here as in the one fermion case.

Solution for problem 11: I only solved the single fermion part. The Hamiltonian here is the same as in problem 3, problem set 5, except for the additional single fermion term

$$\int\mu_1\left(y\right)\mathrm{d}y=\frac{1}{2}\sum_{\alpha,\beta=\pm1}\int\mathrm{d}y\xi_\alpha^\dagger\left(y\right)\sigma_1^{\alpha\beta}\xi_\beta\left(y\right)=\frac{1}{2}\int\mathrm{d}y\left(\xi_{-1}^\dagger\left(y\right)\xi_1\left(y\right)+\xi_1^\dagger\left(y\right)\xi_{-1}\left(y\right)\right) \tag{39}$$

that mixes spin up and down fermions that are in the same position. The most general state that is separated into bosons and fermions and that has a defined fermion number which is 1 is

$$|J\rangle=J\left[a^\dagger\right]\sum_{\alpha=\pm1}\int\mathrm{d}yf_\alpha\left(y\right)\xi_\alpha^\dagger\left(y\right)|0\rangle=|b\rangle\bigotimes\sum_{\alpha=\pm1}\int\mathrm{d}yf_\alpha\left(y\right)\xi_\alpha^\dagger\left(y\right)|0\rangle \tag{40}$$

where $f_\alpha\left(y\right)$ is the position and spin distribution of the fermion. Since the fermions have no kinetic energy term, we may assume the fermion has a defined position, so that $f_\alpha\left(x\right)=c_\alpha\delta\left(x-y\right)$, and

$$|J\rangle=J\left[a^\dagger\right]\sum_{\alpha=\pm1}\int\mathrm{d}yf_\alpha\left(y\right)\xi_\alpha^\dagger\left(y\right)|0\rangle=|b\rangle\bigotimes\sum_{\alpha=\pm1}c_\alpha\xi_\alpha^\dagger\left(y\right)|0\rangle \tag{41}$$

The Hamiltonian is

$$H=\int\frac{\mathrm{d}k}{2\pi}\frac{\hbar^2k^2}{2m}a_k^\dagger a_k+\int\mu_1\left(y\right)\mathrm{d}y+\lambda\int\frac{\mathrm{d}k}{2\pi}\mathrm{d}x\left(a_k^\dagger e^{-ikx}+a_ke^{ikx}\right)\mu_3\left(x\right)\mathrm{d}x \tag{42}$$

We now need to compute $\langle J| H |J\rangle$,

$$\int \mu_1(z)\,\mathrm{d}z\,|J\rangle = |b\rangle \frac{1}{2}\sum_{\gamma,\delta,\alpha}\int \mathrm{d}z\xi_\gamma^\dagger(z)\,\sigma_1^{\gamma\delta}\xi_\delta(z)\,c_\alpha\xi_\alpha^\dagger(y)\,|0\rangle = \tag{43}$$

$$|b\rangle \frac{1}{2}\sum_{\gamma,\delta,\alpha}\int \mathrm{d}z\xi_\gamma^\dagger(z)\,\sigma_1^{\gamma\delta}c_\alpha\delta(z-y)\,\delta_{\alpha\delta}\,|0\rangle = |b\rangle\frac{1}{2}\sum_{\gamma,\alpha}\sigma_1^{\gamma\alpha}c_\alpha\xi_\gamma^\dagger(y)\,|0\rangle\,; \tag{44}$$

$$\Rightarrow\quad \langle J| H |J\rangle = \langle b|\langle 0|\sum_\beta c_\beta^*\xi_\beta(y)\,H\sum_\alpha c_\alpha\xi_\alpha^\dagger(y)\,|0\rangle\,|b\rangle = \tag{45}$$

$$\langle b|\langle 0|\sum_{\alpha\beta}\xi_\beta^\dagger(y)\,c_\beta^* c_\alpha\xi_\alpha(y)\left(\int \mathrm{d}k\frac{\hbar^2k^2}{2m}a_k^\dagger a_k + \frac{\lambda}{2}\int\frac{\mathrm{d}k}{2\pi}\left(a_k^\dagger e^{-iky}+a_k e^{iky}\right)\alpha\right)|b\rangle\,|0\rangle + \tag{46}$$

$$\langle b|\,b\rangle\frac{1}{2}\langle 0|\frac{1}{2}\sum_{\gamma\alpha\beta}\xi_\beta(y)\,c_\beta^*\sigma_1^{\gamma\alpha}c_\alpha\xi_\gamma^\dagger(y)\,|0\rangle = \tag{47}$$

$$\sum_{\alpha\beta}\langle 0|\,\xi_\beta^\dagger(y)\,c_\beta^*c_\alpha\xi_\alpha(y)\,|0\rangle\,\langle b|\left(\int \mathrm{d}k\frac{\hbar^2k^2}{2m}a_k^\dagger a_k + \frac{\lambda}{2}\int\frac{\mathrm{d}k}{2\pi}\left(a_k^\dagger e^{-iky}+a_k e^{iky}\right)\alpha\right)|b\rangle + \tag{48}$$

$$\langle b|\,b\rangle\,\langle 0|\frac{1}{2}\sum_{\gamma\alpha\beta}\xi_\beta(y)\,c_\beta^*\sigma_1^{\gamma\alpha}c_\alpha\xi_\gamma^\dagger(y)\,|0\rangle = \tag{49}$$

$$\delta(0)\,\langle b|\left(\sum_\alpha c_\alpha^*c_\alpha\int \mathrm{d}k\frac{\hbar^2k^2}{2m}a_k^\dagger a_k + \sum_\alpha \alpha c_\alpha^*c_\alpha\frac{\lambda}{2}\int\frac{\mathrm{d}k}{2\pi}\left(a_k^\dagger e^{-iky}+a_k e^{iky}\right)\right)|b\rangle + \tag{50}$$

$$\delta(0)\,\langle b|\,b\rangle\frac{1}{2}\sum_{\alpha\beta}c_\beta^*\sigma_1^{\beta\alpha}c_\alpha = \delta(0)\left[\sum_\alpha|c_\alpha|^2\langle b|\,H_{eff}(\{c_\alpha\},\{c_\alpha^*\})\,|b\rangle + \frac{1}{2}\sum_{\alpha\beta}c_\beta^*\sigma_1^{\beta\alpha}c_\alpha\right] \tag{51}$$

where

$$H_{eff}(\{c_\alpha\},\{c_\alpha^*\}) = \int \mathrm{d}k\frac{\hbar^2k^2}{2m}a_k^\dagger a_k + \frac{\sum_\alpha \alpha\,|c_\alpha|^2}{\sum_\alpha|c_\alpha|^2}\frac{\lambda}{2}\int\frac{\mathrm{d}k}{2\pi}\left(a_k^\dagger e^{-iky}+a_k e^{iky}\right) \tag{52}$$

This needs to be minimized with respect to c_α and $|b\rangle$. To keep normalization we minimize the Lagrange function

$$F(|b\rangle,\langle b|,\{c_\alpha\},\{c_\alpha^*\}) = \left[\langle J| H |J\rangle - E_1\langle b|\,b\rangle - E_2\sum_\alpha|c_\alpha|^2\right]/\delta(0) \tag{53}$$

$$0 = \frac{\partial F}{\partial\langle b|} = \left(\sum_\alpha|c_\alpha|^2 H_{eff}(\{c_\alpha\},\{c_\alpha^*\}) + \frac{1}{2}\sum_{\alpha\beta}c_\beta^*\sigma_1^{\beta\alpha}c_\alpha - E_1\right)|b\rangle \tag{54}$$

$$0 = \frac{\partial F}{\partial c_\alpha^*} = c_\alpha\,\langle b|\int \mathrm{d}k\left[\frac{\hbar^2k^2}{2m}a_k^\dagger a_k + \frac{\lambda}{2}\alpha\left(a_k^\dagger e^{-iky}+a_k e^{iky}\right)\right]|b\rangle + \frac{1}{2}\sigma_1^{\alpha\beta}c_\beta - E_2c_\alpha \tag{55}$$

The equation on $|b\rangle$ is very similar to the one obtained in problem 3, problem set 5

$$\sum_\alpha|c_\alpha|\int \mathrm{d}k\frac{\hbar^2k^2}{2m}a_k^\dagger a_k + \sum_\alpha\alpha\,|c_\alpha|^2\frac{\lambda}{2}\int\frac{\mathrm{d}k}{2\pi}\left(a_k^\dagger e^{-iky}+a_k e^{iky}\right)|b\rangle = \left(E_1 - \frac{1}{2}\sum_{\alpha\beta}c_\beta^*\sigma_1^{\beta\alpha}c_\alpha\right)|b\rangle \tag{56}$$

Redefining

$$E = \left(E_1 - \frac{1}{2}\sum_{\alpha\beta}c_\beta^*\sigma_1^{\beta\alpha}c_\alpha\right)\sum_\alpha|c_\alpha|^2 \tag{57}$$

$$\tilde{c}_\alpha = c_\alpha/\sqrt{\sum_\alpha|c_\alpha|^2} \tag{58}$$

we obtain

$$H_{eff}\left|b\right\rangle = \int \mathrm{d}k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k + \sum_\alpha \alpha \left|\tilde{c}_\alpha\right|^2 \frac{\lambda}{2} \int \frac{\mathrm{d}k}{2\pi} \left(a_k^\dagger e^{-iky} + a_k e^{iky}\right)\left|b\right\rangle = E\left|b\right\rangle \tag{59}$$

As in the HW problem, we define a new bosonic annihilation operator

$$b_k = a_k + \sqrt{\sum_\alpha \left|\tilde{c}_\alpha\right|^2 \alpha} \frac{m\lambda}{\hbar^2 k^2} e^{-iky} \tag{60}$$

Note that $\sum_\alpha \left|\tilde{c}_\alpha\right|^2 \alpha$, which is the spin expectation value, might by negative, but we choose the square root such that $\sqrt{-1} = i$. In terms of b_k (59) takes the form

$$H_{eff}\left|b\right\rangle = \int \mathrm{d}k \frac{\hbar^2 k^2}{2m} \left(b_k^\dagger b_k - \left(\frac{m\lambda}{\hbar^2 k^2}\right)^2 \sum_\alpha \left|\tilde{c}_\alpha\right|^2 \alpha\right) = E\left|b\right\rangle \tag{61}$$

where we have used

$$b_k^\dagger b_k = \left(a_k^\dagger + \sqrt{\sum_\alpha \left|\tilde{c}_\alpha\right|^2 \alpha} \frac{m\lambda}{\hbar^2 k^2} e^{iky}\right)\left(a_k + \sqrt{\sum_\alpha \left|\tilde{c}_\alpha\right|^2 \alpha} \frac{m\lambda}{\hbar^2 k^2} e^{-iky}\right) = \tag{62}$$

$$= a_k^\dagger a_k + \sum_\alpha \left|\tilde{c}_\alpha\right|^2 \alpha \frac{m\lambda}{\hbar^2 k^2}\left(a_k^\dagger e^{-iky} + a_k e^{iky}\right) + \left(\frac{m\lambda}{\hbar^2 k^2}\right)^2 \sum_\alpha \left|\tilde{c}_\alpha\right|^2 \alpha \tag{63}$$

Now it is clear that $\left|b\right\rangle$ must be of the form $\left|b\right\rangle = \prod_{i=1}^N b_{k_i}^\dagger \left|0\right\rangle$ with $N \in \mathbb{N}_0$ and

$$E = \sum_{i=1}^N \frac{\hbar^2 k_i^2}{2m} - \left(\sum_\alpha \left|\tilde{c}_\alpha\right|^2 \alpha\right) \int \frac{\mathrm{d}k}{2\pi} \frac{m\lambda^2}{2\hbar^2 k^2} \tag{64}$$

Now the $\left|b\right\rangle$ dependent term in the fermionic equation can be written as

$$\left\langle b\right| \int \mathrm{d}k \alpha \left(a_k^\dagger e^{-iky} + a_k e^{iky}\right)\left|b\right\rangle = \tag{65}$$

$$\left\langle b\right| \int \mathrm{d}k \alpha \left(\left(b_k^\dagger - \sqrt{\sum_\alpha \left|\tilde{c}_\alpha\right|^2 \alpha} \frac{m\lambda}{\hbar^2 k^2} e^{iky}\right) e^{-iky} + \left(b_k - \sqrt{\sum_\alpha \left|\tilde{c}_\alpha\right|^2 \alpha} \frac{m\lambda}{\hbar^2 k^2} e^{-iky}\right) e^{iky}\right)\left|b\right\rangle = \tag{66}$$

$$-2\alpha \left\langle b\right|\left.b\right\rangle \sqrt{\sum_\alpha \left|\tilde{c}_\alpha\right|^2 \alpha} \int \mathrm{d}k \frac{m\lambda}{\hbar^2 k^2} \tag{67}$$

Defining $\tilde{E} = E_2 - \left\langle b\right| \int \mathrm{d}k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k \left|b\right\rangle$, the fermionic equation may now be written as

$$\left(-2\left\langle b\right|\left.b\right\rangle \sqrt{\sum_\alpha \left|\tilde{c}_\alpha\right|^2 \alpha} \int \mathrm{d}k \frac{m\lambda}{\hbar^2 k^2}\right) \alpha \tilde{c}_\alpha + \frac{1}{2}\sigma_1^{\alpha\beta} \tilde{c}_\beta = \tilde{E}\tilde{c}_\alpha \tag{68}$$

(69)

(70)

(71)

(72)

$$\Rightarrow \tag{73}$$

This is a non linear equation, so I don't know how to generally solve it, but the σ_1 states are solutions since $\sqrt{\sum_\alpha \left|\tilde{c}_\alpha\right|^2 \alpha} = 0$ for these states. These are explicitly

$$\tilde{E}_\pm = \pm\frac{1}{2},\ \tilde{\boldsymbol{c}}_\pm = \begin{pmatrix} (c_1)_\pm \\ (c_2)_\pm \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} \pm 1 \\ 1 \end{pmatrix} \tag{74}$$

The fermionic states are thus just states of σ_1 localized at y, $|\pm, y\rangle = \frac{1}{\sqrt{2}}\left(\pm\xi_{-1}^{\dagger}(y) + \xi_1^{\dagger}(y)\right)|0\rangle$. The value of the energy functional is

$$\langle J|\,H\,|J\rangle/\delta(0) = \left[\sum_{\alpha}|c_\alpha|^2\langle b|\,H_{eff}(\{c_\alpha\},\{c_\alpha^*\})\,|b\rangle + \frac{1}{2}\sum_{\alpha\beta}c_\beta^*\sigma_1^{\beta\alpha}c_\alpha\right] = \tag{75}$$

$$= E \pm \frac{1}{2} \tag{76}$$

where the infinite energy part drops because $\left(\sum_\alpha|\tilde{c}_\alpha|^2\alpha\right) = 0$ when $\boldsymbol{c}$ is an eigenstate of σ_1. The minimum is obtained with $-1/2$ and $E = 0$, with the states $|b\rangle = |0\rangle$ for the bosonic part and $|-, y\rangle$ for the fermionic part. The variational ground state is

$$|J\rangle = |0\rangle\,|-, y\rangle = |0\rangle\bigotimes\frac{1}{\sqrt{2}}\left(\xi_{-1}^{\dagger}(y) + \xi_1^{\dagger}(y)\right)|0\rangle \tag{77}$$

It is easy to verify directly that with this $|J\rangle$, $\langle J|\,H\,|J\rangle = -1/2$.

Problem 12: Consider the Hamiltonian

$$H = \frac{p_x^2}{2m_x} + \frac{p_y^2}{2m_y} + \frac{k}{2}\left(x^2 + y^2\right) + \alpha xy \tag{78}$$

and assume that $m_y \gg m_x$. Find the energy levels and the corresponding wave functions using the Born-Oppenheimer approximation. This problem has an exact solution. Find it and compare with the BO result.

Solution 12: Exact solution through normal modes: We find the classic normal modes,

$$H = \frac{1}{2}\boldsymbol{p}^t M^{-1}\boldsymbol{p} + \frac{1}{2}\boldsymbol{x}^t K\boldsymbol{x} \tag{79}$$

$$M^{-1} = \begin{pmatrix} m_x^{-1} & 0 \\ 0 & m_y^{-1}\end{pmatrix};\ K = \begin{pmatrix} k & \alpha \\ \alpha & k\end{pmatrix} \tag{80}$$

First swallow the M^{-1} into the ps. It comes out in the xs. Then Diagonalize $M^{-1/2}KM^{-1/2}$ with an orthogonal matrix. To get new canonical coordinates in which the two HOs are decoupled. The frequencies are

$$\omega_\pm^2 = \frac{k(m_x + m_y) \pm \sqrt{k^2(m_x - m_y)^2 + 4\alpha^2 m_x m_y}}{2m_x m_y} = \frac{1}{2m_x}\left[k\left(\frac{m_x}{m_y} + 1\right) \pm \sqrt{k^2\left(1 - \frac{m_x}{m_y}\right)^2 + 4\alpha^2\frac{m_x}{m_y}}\right] \tag{81}$$

$$\approx \frac{k}{2m_x}\left[\left(\frac{m_x}{m_y} + 1\right) \pm \left(1 + \left(2\frac{\alpha^2}{k^2} - 1\right)\frac{m_x}{m_y}\right)\right] \approx \begin{cases}\frac{k}{m_x} = \omega^2 & + \\ \frac{k}{m_y}\left(1 - \frac{\alpha^2}{k^2}\right) = \Omega^2 & -\end{cases} \tag{82}$$

Born Oppenheimer approximation:

1. Identifying fast part: $m_y \gg m_x$

$$H = \frac{p_x^2}{2m_x} + \frac{p_y^2}{2m_y} + \frac{k}{2}\left(x^2 + y^2\right) + \alpha xy \tag{83}$$

$$H_{fast} = \frac{p_x^2}{2m_x} + \frac{1}{2}m_x\left(\sqrt{\frac{k}{m_x}}\right)^2\left(x + \frac{\alpha}{k}y\right)^2 \tag{84}$$

$$H = \frac{p_y^2}{2m_y} + \frac{1}{2}k\left(1 - \frac{\alpha^2}{k^2}\right)y^2 + H_{fast} \tag{85}$$

2. Solving $H_{fast}(x;y)\,\phi(x;y) = \varepsilon(y)\,\phi(x;y)$: this is a shifted HO with the parameter y determining the shift

$$\varepsilon_n(y) = \hbar\omega\left(n+\frac{1}{2}\right) \tag{86}$$

$$\phi_n(x;y) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega(x+\alpha y/k)^2/2\hbar} H_n\left(\sqrt{\frac{m\omega}{\hbar}}\left(x+\frac{\alpha y}{k}\right)\right) \tag{87}$$

$$\omega = \sqrt{k/m_x} \tag{88}$$

3. Solving:

$$\left[\frac{1}{2m_y}\left(p_y - iA_n(y)\right)^2 + \frac{1}{2}k\left(1-\frac{\alpha^2}{k^2}\right)y^2 + \varepsilon_n(y)\right]\xi_{n,k}(y) = E_{n,k}\xi_{n,k}(y) \tag{89}$$

Here $A_n = 0$ since $A_n = \langle\phi_n|\,\partial_y\,|\phi_n\rangle$ is imaginary while ϕ_n are real. What remains is also a simple HO

$$\left[\frac{p_y^2}{2m_y} + \frac{1}{2}k\left(1-\frac{\alpha^2}{k^2}\right)y^2 + \hbar\omega\left(n+\frac{1}{2}\right)\right]\xi_{n,k}(y) = E_{n,k}\xi_{n,k}(y) \tag{90}$$

The energies are

$$E_{n,k} = \hbar\Omega\left(k+\frac{1}{2}\right),\ \Omega = \sqrt{\frac{k}{m_y}\left(1-\frac{\alpha^2}{k^2}\right)} + \hbar\omega\left(n+\frac{1}{2}\right) \tag{91}$$

and the functions are the Ω, m_y wave function. In the limit $m_y \gg m_x$ the exact energies are precisely the Born Oppenheimer energies.

Problem 6:

References