Quantum Solutions

1. (a) Let $\{|\psi_n\rangle\}$ $(n = 1, 2, \ldots)$ be an orthonormal basis of $\mathcal{H}$ consisting of eigenvectors of A. We have

$$A = \sum_n \lambda_n \, |\psi_n\rangle\langle\psi_n| \quad ,$$

where $A\,|\psi_n\rangle = \lambda_n|\psi_n\rangle$. Writing $\lambda_n = |\lambda_n|\mathrm{e}^{i\theta_n}$, we define

$$U = \sum_n \mathrm{e}^{i\theta_n} \, |\psi_n\rangle\langle\psi_n|$$

and

$$B = \sum_n |\lambda_n| \, |\psi_n\rangle\langle\psi_n| \quad .$$

The orthonormality of the basis then gives $A = UB$.

(b) Let E_n $(n = 0, 1, \ldots, N-1)$ denote the eigenvalues of H, with $E_0 \le E_1 \le \cdots \le E_{N-1}$. Then $\mathrm{Tr}(H) = \sum_n E_n \ge N E_0$. But we also have $\mathrm{Tr}(H) = \mathrm{Tr}(A) - \mathrm{Tr}(B^2) \le \mathrm{Tr}(A)$, since the Hermiticity of B implies $\mathrm{Tr}(B^2) \ge 0$. Putting these two inequalities together yields the desired result. An explicit example (with $H \ne 0$) is given by $A = \lambda\, I$ (λ real) and $B = 0$.

2. (a) The reduced radial Schrödinger equation for the system reads $H_\ell\, u_{n,\ell}(r) = E_{n,\ell}\, u_{n,\ell}(r)$, where

$$H_\ell = -\frac{\hbar^2}{2M}\frac{d^2}{dr^2} + \frac{\hbar^2 \ell(\ell+1)}{2\,Mr^2} + V(r) \quad ,$$

and M is the mass of the particle. By the Variational Theorem we have $E_{0,\ell} \le \langle H_\ell\rangle_{0,\ell+1}$ (the expectation value of H_ℓ in the reduced radial wavefunction $u_{0,\ell+1}(r)$). But $H_\ell = H_{\ell+1} - A$, where $A = \frac{\hbar^2(2\ell+1)}{2\,Mr^2}$. This, along with $\langle H_{\ell+1}\rangle_{0,\ell+1} = E_{0,\ell+1}$ and $\langle A\rangle_{0,\ell+1} > 0$ (which follows since A is everywhere positive), then yields the desired strict inequality.

(b) Since $V(x) \to 0$ as $x \to \pm\infty$, the Variational Theorem tells us that the system possesses a bound state if and only if there exists a square-integrable function $\psi(x)$ such that $\langle H\rangle_\psi < 0$, where H is the (non-relativistic) Hamiltonian operator of the system. To this end, consider a one-parameter family of "trial wavefunctions" of the form (say) $\psi(x;\alpha) = N\,\alpha^{1/4}\,\mathrm{e}^{-\alpha x^2/2}$, where $\alpha > 0$ and N is a normalization constant ($\langle\psi|\psi\rangle = 1$). By dimensional analysis, N is independent of α, and the expectation value of the kinetic energy in the state $\psi(x;\alpha)$ is equal to $c\,\hbar^2\alpha/M$, where $c > 0$ is independent of α, and M is the mass of the particle. (Both N and c are dimensionless.) The expectation value of the potential energy is easily seen to be $(\lambda+\mu)\,|N|^2\sqrt{\alpha}\,\mathrm{e}^{-\alpha b^2} < 0$. Thus, $\langle H\rangle < 0$ in the state $\psi(x;\alpha)$ if and only if $z\sqrt{\alpha} < \mathrm{e}^{-\alpha b^2}$, where $z = c\,\hbar^2/M\,|\lambda+\mu|\,|N|^2$ is independent of α. By choosing α small enough, this can always be satisfied. Finally, for $\lambda\cdot\mu < 0$ we have one "attractive" and one "repulsive" delta-function in $V(x)$, which (like the single attractive delta-function) cannot hold more than one bound state.

3. (a) (i) The ground state energy to first-order in λ is given by

$$E_0 = \frac{1}{2}\,\hbar\,\omega + \lambda \int_{-\infty}^{+\infty} |x|\,|\psi_0^{(0)}(x)|^2\,\mathrm{d}x \quad ,$$

where $\psi_0^{(0)}(x) = (\frac{\alpha}{\pi})^{1/4}\,\mathrm{e}^{-\alpha x^2/2}$ $(\alpha = M\omega/\hbar)$ is the ground state wavefunction of the harmonic oscillator (that is, $\lambda = 0$) potential. The integral is easily done, yielding $E_0 = \frac{1}{2}\,\hbar\,\omega + \lambda\sqrt{\frac{\hbar}{\pi\,M\,\omega}}$.

(ii) For all λ we have $V(x) \to \infty$ as $x \to \pm\infty$. When $\lambda > 0$, $V(x)$ is a "single-well" potential which becomes "infinitely narrow" as $\lambda \to \infty$. Thus, $(E_1 - E_0) \to \infty$ in this limit. When $\lambda < 0$, $V(x)$ is a "double-well" potential whose two minima get deeper and further apart as λ increases, so that we obtain two completely isolated (identical) wells as $\lambda \to -\infty$ (tunneling is completely suppressed). Thus, $(E_1 - E_0) \to 0$ in this limit. (That is, the ground state becomes doubly degenerate.)

(b) $E_s^{(1)} = \langle \psi_s^{(0)} | H_1 | \psi_s^{(0)} \rangle = \mu$. We also have

$$E_s^{(2)} = \sum_{t \neq s} \frac{|\langle \psi_s^{(0)} | H_1 | \psi_t^{(0)} \rangle|^2}{(E_s^{(0)} - E_t^{(0)})} = \frac{\mu^2}{\Delta} \left(\sum_{t=0}^{s-1} \frac{1}{(s-t)} - \sum_{t=1}^{\infty} \frac{1}{t} \right) ,$$

where $\Delta = E_{n+1}^{(0)} - E_n^{(0)}$. But the "harmonic series" $\sum_{t=1}^{\infty} \frac{1}{t}$ diverges.

4. (a) The two possible results of the measurement are the eigenvalues of A, which are $\pm\lambda$. The corresponding eigenvectors are given by $|\psi_\pm\rangle = \frac{1}{\sqrt{2}} (|1\rangle \pm |2\rangle)$. If the qubit is in the state $|\psi_\alpha\rangle$, the probability of obtaining the result $+\lambda$ is $|\langle \psi_\alpha | \psi_+ \rangle|^2 = \cos^2(\pi\alpha)$, and the probaility of obtaining $-\lambda$ is $|\langle \psi_\alpha | \psi_- \rangle|^2 = \sin^2(\pi\alpha)$. Thus, the fractions of the total measurements which yield these results are given by $\int_0^1 p(\alpha) \, |\langle \psi_\alpha | \psi_\pm \rangle|^2 \, \mathrm{d}\alpha = 1/2$ (an equal amount of $+\lambda$'s and $-\lambda$'s).

(b) If the lesser result $(-\lambda)$ is obtained, the state immediately after the measurement is $|\psi_-\rangle$. The energy eigenstates of the system are $|1\rangle$ and $|2\rangle$, with eigenvalues $+\mu$ and $-\mu$, respectively. Thus, if the measurement is performed at time $t = 0$, the state of the sytem at time $t \geq 0$ is given by

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} \left(\mathrm{e}^{-i\mu t/\hbar} \, |1\rangle - \mathrm{e}^{i\mu t/\hbar} \, |2\rangle \right) .$$

5. (a) The Hamiltonian operator of the system (in the position representation) is given by $H = -\frac{\hbar^2}{2M} \left(\nabla_1^2 + \nabla_2^2 \right) + V(\vec{r}_1, \vec{r}_2)$. Separation of variables is achieved by transforming to the two-particle center-of-mass and relative coordinates, $\vec{R} = \frac{1}{\sqrt{2}}(\vec{r}_1 + \vec{r}_2)$ and $\vec{r} = \frac{1}{\sqrt{2}}(\vec{r}_1 - \vec{r}_2)$. More specifically, we now have

$$H = -\frac{\hbar^2}{2\,M} \left(\nabla_{\vec{R}}^2 + \nabla_{\vec{r}}^2 \right) + \frac{1}{2} \, M \, \omega^2 \, R^2 + \frac{\hbar^2}{M \, r^2} + \frac{1}{2} \, M \, \omega^2 \, r^2 ,$$

where $R = |\vec{R}\,|$ and $r = |\vec{r}\,|$. Hence, the center-of-mass contribution to the ground state energy is $\frac{3}{2} \, \hbar \, \omega$ (the ground state energy of a 3D harmonic oscillator). The "relative" contribution is $\frac{5}{2} \, \hbar \, \omega$, which is the 3D harmonic oscillator energy with radial quantum number $n = 0$ and orbital angular momentum quantum number $\ell = 1$ (the $\frac{1}{r^2}$ term in H acts as an "effective" $\ell = 1$ angular momentum barrier term for the relative coordinate). Thus, the total ground state energy of our system is $4 \, \hbar \, \omega$. The ground state wavefunction only depends on r and R, and is given by

$$\Psi(r, R) = N \, r \, \mathrm{e}^{-\alpha r^2/2} \, \mathrm{e}^{-\alpha R^2/2} ,$$

where N is a normalization constant, and $\alpha = M \, \omega / \hbar$. This is the product of the standard 3D harmonic oscillator radial wavefunctions $\mathcal{R}_{n=0,\ell=0}(R)$ and $\mathcal{R}_{n=0,\ell=1}(r)$. (Note that the $\ell = 1$ spherical harmonics *do not* appear here.)

(b) Two observables are simultaneously measurable if and only if their associated Hermitian operators commute. Hence, we need to find all pairs of commuting operators in the set W. To this end, recall that (for all i, j, k) we have $[L_i, L_j] = \mathrm{i} \, \hbar \sum_k \epsilon_{ijk} L_k$ (similarly for $[S_i, S_j]$), $[L^2, L_i] = [S^2, S_i] = [S_i, L_j] = 0$, $J_i = L_i + S_i$, and $J^2 = L^2 + S^2 + 2 \, \vec{S} \cdot \vec{L}$. From this, we see that the only pairs in W which *don't* commute are (L_i, L_j) , (S_i, S_j), (J_i, J_j), (J_i, S_j) and (J_i, L_j) (in each case for all $i \neq j$). Finally, we also see that $[J^2, \vec{S} \cdot \vec{L}] = 0$.