QM II: Übungszettel 7
(Abgabetermin: 04.06.2014)

Variational method (20 pts)

Consider a normalized test function $\tilde{\Phi}(x)$ that is orthogonal to the exact ground state wavefunction, $\langle\tilde{\Phi}|\Phi_0\rangle = 0$.

(a) Show that

$$\langle\tilde{\Phi}|\hat{\mathbf{H}}|\tilde{\Phi}\rangle \geq E_1 \,,$$

where E_1 is the true eigenenergy of the first excited state.

(b) We now allow only for linear variations of the test function, that is, we fix an orthonormal basis $\{|\varphi_i\rangle\}$ such that $|\tilde{\Phi}\rangle = \sum_{i=1}^{N} c_i|\varphi_i\rangle$ and vary only the c_i. Show that in this case you can write the variational problem as a standard matrix eigenvalue problem, $\mathbf{H}\vec{c} = \mathcal{E}\vec{c}$. How many eigenvectors $\vec{c}$ and eigenvalues $\mathcal{E}$ will the solution of this eigenvalue problem yield?

(c) Consider the function

$$\tilde{\Phi}(x) = \alpha_0\tilde{\Phi}_0(x) + \alpha_1\tilde{\Phi}_1(x) \,,$$

where $|\tilde{\Phi}_j\rangle = \sum_{i=1}^{N} c_i^j|\varphi_i\rangle$ with c_i^j the ith element of the jth eigenvector from problem (b). Show that normalization of $\tilde{\Phi}(x)$ implies $|\alpha_0|^2 + |\alpha_1|^2 = 1$ and

$$\langle\tilde{\Phi}|\hat{\mathbf{H}}|\tilde{\Phi}\rangle = \mathcal{E}_0 - |\alpha_0|^2(\mathcal{E}_1 - \mathcal{E}_0) \,.$$

Why can you conclude that $\mathcal{E}_1 \geq E_1$? Can you generalize the argument to $\mathcal{E}_j \geq E_j$, $j = 2, 3, \ldots$? If so, why?

Application of the variational method (30 pts)

(a) Consider the square well potential

$$V(x) = \begin{cases} 0 & \text{if} \quad |x| < a \\ \infty & \text{if} \quad a \leq |x| \end{cases}$$

What are the exact ground state wavefunction and energy? Calculate the energy for the test function

$$\psi(x) = a^2 - x^2 \,.$$

Show that the result of this simple ansatz differs by only 1.3% from the exact value. Give a reason why the ansatz works so well, that is, explain which properties are shared by the test function and the true ground state wavefunction.

(b) Now consider a family of functions

$$\psi_\lambda(x) = |a|^\lambda - |x|^\lambda$$

with real parameter λ. Determine the optimal $\psi_\lambda(x)$ by variation of λ. By how much differs the minimal energy that you get this way from the true ground state energy?

(c) Consider the hydrogen atom, i.e., the Hamiltonian $\hat{\mathbf{H}}$ for an electron with charge $-e_0$ and mass m that moves in the Coulomb potential of a nucleus with charge Ze_0. Choose the ground state wavefunction of the three-dimensional harmonic oscillator with potential $m\omega r^2/2$ as your test function,

$$\psi_0(\vec{x}) = \left(\frac{m\omega}{\hbar\pi}\right)^{3/4} \exp\left[-\frac{m\omega}{2\hbar}r^2\right] \,.$$

Find an optimal estimate for the ground state energy of the hydrogen atom by variation of ω. Compare the result to the true ground state energy.
Hint: It is useful to first show that $\langle\psi_0|\hat{\mathbf{H}}|\psi_0\rangle = \frac{3}{4}\hbar\omega - \frac{2Ze_0^2}{\hbar}\sqrt{\hbar\omega m/\pi}$.