PHY 304, II-Semester 2023/24, Assignment 3

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Due-date: 11. Feb. 2024

(1) Integrations in atomic physics: [8 pts] In the week 3 and 4 material, you will see a few high dimensional integrations that frequently arise in atomic and molecular physics.[1] Feel free to provide a solution that is a hybrid between pen/paper and `mathematica`, but we need you to clearly discuss all steps that break down the original high dimensional integral into final 1D pieces.

(a) Find $\langle \frac{1}{r} \rangle$, $\langle \frac{1}{r^2} \rangle$ and $\langle \frac{1}{r^3} \rangle$ in a Hydrogen state $|\, n\ell m \,\rangle$ [Eq. (4.91)], used in section (7.3.1) [4pts]. *Hints: In these integrations you (and mathematica) may be challenged by integrations over Laguerre polynomials $L_q^p(r)$ (with arbitrary p, q) times further functions of r. We shall defeat those with a few cunning tricks, that make the problem at first much more complicated looking, but in the end do help because they reduce the integration to one over polynomials and exponentials, which is easy. At the core are the generating functions*[2] *for Laguerre polynomials, which are*

$$U_p(s,\rho) = \frac{(-s)^p}{(1-s)^{p+1}} \exp\left(-\frac{\rho s}{1-s}\right) = \sum_{q=p}^{\infty} \frac{L_q^p(\rho)}{q!} s^q. \tag{1}$$

Proceed as follows: (i) Where you encounter Laguerre polynomials $L_q^p(\rho)^2$ in the integration, write $U_p(s,\rho)U_p(t,\rho)$ instead. (ii) Integrate, you may use

$$\int_0^\infty du\; e^{-u}\; u^n = n! \tag{2}$$

and will reach a function of s, t. (iii) Using the expansion

$$(1-x)^{-n} = \sum_{a=0}^{\infty} \binom{n+a-1}{a} x^a, \tag{3}$$

where the brackets denote a Binomial coefficient, write the result as a power series in s, t. (iv) Identify which single one of the coefficients of this power series gives you the integral you were originally after. (v) You have to do this whole program only once, insertion of the right coefficients in the end gives you all three integrals sought. To get your final results into the right shape, you also need some further identities involving Binomial coefficients

$$\sum_{r=0}^{m} \binom{n+r}{r} = \binom{n+m+1}{m} \tag{4}$$

[1] There will be no problem to do this question prior to having gone through the week 4 material.

[2] Generating function means, that the polynomial that we care about can be viewed as the coefficients in a power series of said function.

and

$$\sum_{a=0}^{k-1}(k-a)^2\binom{j+a}{a} = \frac{(j+2k+1)(j+k+1)!}{(k-1)!(j+3)!}. \tag{5}$$

(b) Evaluate the overlapp integral $I = \int d^3\mathbf{r}\,\phi_{100}(\mathbf{r})\phi_{100}(\mathbf{r}')$ in Eq. (7.110), where ϕ_{100} is the Hydrogen ground-state wavefunction [2 pts].

(c) Evaluate the direct and exchange integrals in Eq. (7.113), Eq. (7.114). [2 pts]

$$I_{\text{dir}} = a_0 \int d^3\mathbf{r}\,\phi_{100}(\mathbf{r})\frac{1}{r'}\phi_{100}(\mathbf{r}) = \frac{a_0}{R} - \left(1+\frac{a_0}{R}\right)e^{-2R/a_0}, \tag{6}$$

$$I_{\text{ex}} = a_0 \int d^3\mathbf{r}\,\phi_{100}(\mathbf{r})\frac{1}{r}\phi_{100}(\mathbf{r}') = \left(1+\frac{a_0}{R}\right)e^{-R/a_0}. \tag{7}$$

(2) Potential well with linear slope: [6 pts] A particle of mass m is trapped in a potential well of the form $V(x) = \beta|x|$ with $\beta > 0$.

(a) Sketch this potential and the expected shape and symmetries of the ground-state wavefunction and justify your answers [1pts].

(b) In oder to find the ground-state, decide on your own trial wavefunction for the variational method with at least one variational parameter and justify your choices. Using that trial wavefunction, find an approximation to the ground-state wavefunction and energy [3pts].

(c) The exact solution[3] of this problem has a ground-state energy

$$E_g = 1.01879\left(\frac{\beta^2}{2m\hbar^2}\right)^{1/3} \tag{8}$$

and wavefunction

$$\phi_g(x) = 1.21954\left(\frac{2m\beta}{\hbar^2}\right)^{1/6} \times \text{Ai}\left[\left(\frac{2m\beta}{\hbar^2}\right)^{1/3}|x| - 1.01879\right], \tag{9}$$

where Ai denotes the Airy function (of the first kind). Compare your solution for the energy with Eq. (8) and discuss why/how the variational method has helped. Similarly compare your trial solution with the true solution in the same figure using e.g. `mathematica` for several different parameters, and discuss your achievements [2pts].

[3]Please do not use this kind of function as trial function in (b).

(3) Higher order perturbation theory: [8 pts] Following our approach of "week 2", derive the third order correction of the energy $\lambda^3 E_n^{(3)}$ and the second order correction to the quantum states $\lambda^2 |\, \psi_n^{(2)} \,\rangle$.

(4) Perturbation theory versus exact calculation: [8 pts] Consider the Hamiltonian in matrix form (basis $\{|\, 1 \,\rangle, |\, 2 \,\rangle, \cdots |\, 6 \,\rangle\}$)

$$\hat{H} = \begin{bmatrix} E_a & 0 & \kappa & 0 & 0 & 0 \\ 0 & E_a & 0 & 0 & -\kappa & 0 \\ \kappa & 0 & E_a & 0 & 0 & 0 \\ 0 & 0 & 0 & E_b & 0 & 2\kappa \\ 0 & -\kappa & 0 & 0 & E_b & 0 \\ 0 & 0 & 0 & 2\kappa & 0 & E_b \end{bmatrix}, \tag{10}$$

for real and positive E_a, E_b, κ, let $E_b > E_a$.

(a) Assuming $\kappa \ll E_a, E_b$, use the appropriate type of perturbation theory to find all perturbed eigenvalues and eigenvectors to order κ [2pts].

(b) Now going to the inverse limit of $\kappa \gg |E_b - E_a|$, use the appropriate type of perturbation theory to find all perturbed eigenvalues and eigenvectors to order $|E_b - E_a|$ [3pts]. *Hint: First simplify the Hamiltonian by re-adjusting the zero of energy. Then change into the eigenbasis appropriate for large κ.*

(c) Finally, checkout the spectrum over the whole range of $0 < \kappa < 10$ adapting `Assignment3_program_draft_v2.nb` at the XXX in the code. Discuss your results. Also discuss the behavior of eigenvalues across the whole range of κ and check out how one interesting eigenvector changes with κ [3pts].

(5) Zeeman effect: Bonus (= no extra marks and no penalties for not doing this question. But nice learning in preparation for e.g. PHY402) The script `Assignment3_program_bonus_draft_v1.nb` is set up to provide the calculation for the Zeeman effect for all field strengths, as in example 58. Consider only the $|\, 2p \,\rangle$ state of Hydrogen. We shall use two different bases for the angular momentum, the total angular momentum basis

$$\begin{aligned} \mathcal{B}_{tot} = \{ &|\, j = \frac{3}{2}, m_j = \frac{3}{2} \,\rangle, |\, j = \frac{3}{2}, m_j = \frac{1}{2} \,\rangle, |\, j = \frac{3}{2}, m_j = -\frac{1}{2} \,\rangle, \\ &|\, j = \frac{3}{2}, m_j = -\frac{3}{2} \,\rangle, |\, j = \frac{1}{2}, m_j = \frac{1}{2} \,\rangle, |\, j = \frac{1}{2}, m_j = -\frac{1}{2} \,\rangle\} \end{aligned} \tag{11}$$

and the separate basis

$$\begin{aligned} \mathcal{B}_{sep} = \{ &|\, m_\ell = 1, m_s = \frac{1}{2} \,\rangle, |\, m_\ell = 1, m_s = -\frac{1}{2} \,\rangle, |\, m_\ell = 0, m_s = \frac{1}{2} \,\rangle, \\ &|\, m_\ell = 0, m_s = -\frac{1}{2} \,\rangle, |\, m_\ell = -1, m_s = \frac{1}{2} \,\rangle, |\, m_\ell = -1, m_s = -\frac{1}{2} \,\rangle\} \end{aligned} \tag{12}$$

(a) Revise QM-I, section 4.8., on addition of angular momenta, to figure out what the above means, and based on rules there and QM-II Eqns. (7.84) and (7.85) set up a basis transformation matrix $\underline{\underline{O}}$ such that $\mathcal{B}_{tot} = \underline{\underline{O}}\mathcal{B}_{sep}$. Implement that matrix at one of the XXX in the code, you may use the defined prefactors. [2 pts]

(b) We have already used the Hamiltonians $\hat{H}_a$, $\hat{H}_b$, $\hat{H}_c$ from Eq. (7.81) plus Darwin Term and relativistic corrections to find the fine-structure energies in Eq. (7.74). Use that to set up the Matrix Representation of the combination of all these terms in the basis $\mathcal{B}_{tot}$ at XXX for $\hat{H}_{fs}$. [2 pts]

(c) We shall ignore $\hat{H}_e$ in Eq. (7.81) but have to add $\hat{H}_d$. This one is easiest expressed in the basis $\mathcal{B}_{sep}$, insert XXX for $\hat{H}_{mag}$. [2 pts]

(d) Now combine both contributions into a total Hamiltonian $\hat{H}_{tot} = \hat{H}_{fs} + \hat{H}_{mag}$ at another XXX and execute all the subsequent lines of code that should find eigenvalues and eigenvectors as a function of magnetic field. Discuss all the plots. In particular relate the eigenvectors to the labels of lines in the figures. [3 pts]