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Problem 4.1: Hydrogen Atom – Lowest States

[**Written** | 4 pt(s)]

ID: ex_hydrogen_atom_lowest_states:fqt2425

Learning objective

In this exercise, we will revisit the hydrogen atom problem and determine the size of the atoms where electrons occupy the lower states.

Consider the wave functions of the Hydrogen atom $\psi_{n,\ell,m}$,

$$\psi_{n,l,m}(r,\theta,\varphi) = R_{n,l}(r)Y_{lm}(\theta,\varphi), \tag{1}$$

$$R_{nl}(r) = -N_{nl}(2\kappa r)^l e^{-\kappa r} L^{2l+1}_{n-l-1}(2\kappa r), \tag{2}$$

$$N_{nl} = \left(\frac{1}{a}\right)^{3/2} \frac{2}{n^2(n+l)!}\sqrt{\frac{(n-l-1)!}{(n+l)!}}, \tag{3}$$

where $\kappa = 1/an$, and a refers to the Bohr radius, and L^k_p are the Laguerre polynomials.

a) Write explicitly the $1s$, $2s$, and $2p_z$ wave functions, which correspond to the set of quantum numbers $\{n,\ell,m\} = \{1,0,0\}$, $\{2,0,0\}$, and $\{2,1,0\}$, respectively. **2**pt(s)

b) Determine the expectation value of the radial components r, r^2 and $1/r$ in the ground state (i.e. the $1s$ state) and the $2p_z$ state. Deduce the size of the atom in each of these states. **2**pt(s)

Problem 4.2: One-dimensional lattice and Bloch waves

[**Oral** | 8 pt(s)]

ID: ex_1d_bloch_theorem:fqt2425

Learning objective

The purpose of this exercise is to use your knowledge of translational symmetry and the Bloch's theorem to obtain the so-called Wannier functions. This representation of Bloch states is particularly useful in the context of solid-state physics.

Note: Bloch's theorem will be discussed this week (week of Nov 4) in the lecture.

Consider a one-dimensional lattice with lattice sites at R_m and periodic potential $V(r) = V(r+R_m)$ (without loss of generality the origin of the coordinate system is at either one of the lattice sites). Due to Bloch's theorem the eigenfunctions of the Hamilton operator H can be written in the form $\psi_k(r) = e^{ikr}u_k(r)$, where $u_k(r)$ is lattice periodic (i.e. $u_k(r+R_m) = u_k(r)$), k is located in the first Brillouin zone ($|k| \leq \pi/a$) and a is the distance between two lattice sites.

a) Show that for a lattice with N sites, k has exactly N discrete values. **2**pt(s)

   Hint: Explore the periodic boundary conditions of $\psi_k(r)$, i.e., $\psi_k(r+L) = \psi_k(r)$ if the one-dimensional lattice has length $L = Na$.

b) Using Bloch's theorem (i) show that $E_k = E_{-k}$ and then (ii) that $\psi_k^*(r) = \psi_{-k}(r)$, where E_k are the corresponding energy eigenvalues of the Hamiltonian H. **2**pt(s)

Now assume that the length of the lattice tends to infinity ($L \to \infty$). The Bloch wave functions then obey the orthogonality relation,

$$\int dr \psi_k^*(r)\, \psi_{k'}(r) = \Omega_B \delta(k - k')\,, \tag{4}$$

where Ω_B is the volume of the first Brillouin zone. Now, consider the expansion of the wave functions,

$$\psi_k(r) = \sum_m w(r - R_m)\, e^{ikR_m}, \quad \text{with } w(r-R) = \frac{1}{\Omega_B}\int_{\Omega_B} dk \psi_k(r) e^{-ikR} \tag{5}$$

where the R_m-summation runs over all lattice sites and the k−integration extends along the Brillouin zone.

c) Without using the definition of w, show that $\psi_k(r)$ in the given representation fulfils Bloch's theorem. **2**pt(s)

d) Show that for different R_m the functions w are orthogonal to each other (these functions, which are localized around the lattice sites R_m, are called Wannier functions). **2**pt(s)

Problem 4.3: Angular momentum and rotations

[**Oral** | 8 pt(s)]

ID: ex_angular_momentum:fqt2425

Learning objective

Although we already investigated the angular momentum commutation relations in the first problem list, here we will do this from a different perspective, i.e., by seeing angular momentum operators as the generators of infinitesimal rotations.

Note: Theory of angular momentum and rotations will be discussed this week (week of Nov 4) in the lecture.

Consider the angular momentum operator $\mathbf{L} = \mathbf{r} \times \mathbf{p}$. In the lecture it was shown that $\mathbf{L}$ is the infinitesimal generator of rotations such that rotations around some axis $\mathbf{n}$ with $\mathbf{n}^2 = 1$ about some angle ω can be written as $U_{\boldsymbol{\omega}} = \exp(-i\omega \mathbf{L}\cdot\mathbf{n}/\hbar)$. If $U_{\boldsymbol{\omega}}$ is the operator performing a rotation around some axis $\boldsymbol{\omega} = \omega\mathbf{n}$ in the Hilbert space, i.e. $|\phi_{\boldsymbol{\omega}}\rangle = U_{\boldsymbol{\omega}} |\phi\rangle$; a *scalar* operator S transforms like

$$U_{\boldsymbol{\omega}}^\dagger\, S\, U_{\boldsymbol{\omega}} = S\,, \tag{6}$$

and a *vector* operator $\mathbf{X}$ transforms like

$$U_{\boldsymbol{\omega}}^\dagger\, \mathbf{X}\, U_{\boldsymbol{\omega}} = R_{\boldsymbol{\omega}}\, \mathbf{X}\,, \tag{7}$$

where $R_{\boldsymbol{\omega}}$ is the usual rotation matrix in three dimensions around some axis $\boldsymbol{\omega}$.

a) Show that for a scalar operator S, $[\mathbf{L}, S] = 0$. **2**pt(s)

b) Show that for a vector operator $\mathbf{X}$ it is $[L_i, X_j] = i\hbar\varepsilon_{ijk}X_k$. **2**pt(s)
Hint: Use the representation $(\mathcal{R}_{\boldsymbol{\omega}})_{ij} = [1 - \cos(\omega)]\hat{\omega}_i\hat{\omega}_j + \cos(\omega)\,\delta_{ij} - \sin(\omega)\,\varepsilon_{ijk}\hat{\omega}_k$ for the rotation matrix and linearize (7) for small ω.

c) Using that $\mathbf{r}$ and $\mathbf{p}$ are vector operators, show that $\mathbf{L}$ is also a vector operator. **2**pt(s)
Hint: Consider the components of $U_{\boldsymbol{\omega}}^\dagger\,\mathbf{r}\times\mathbf{p}\,U_{\boldsymbol{\omega}}$ and show that $U_{\boldsymbol{\omega}}^\dagger\,\mathbf{r}\times\mathbf{p}\,U_{\boldsymbol{\omega}} = U_{\boldsymbol{\omega}}^\dagger\,\mathbf{r}\,U_{\boldsymbol{\omega}} \times U_{\boldsymbol{\omega}}^\dagger\,\mathbf{p}\,U_{\boldsymbol{\omega}}$.

d) Show that $[\mathbf{L}, \mathbf{p}\cdot\mathbf{r}] = 0$ on the one hand by explicitely calculating the commutator and on the other hand by showing that $\mathbf{p}\cdot\mathbf{r}$ is a scalar operator. **2**pt(s)