PHY 742 Quantum Mechanics II
1-1:50 AM MWF Olin 103

Plan for Lecture 20

Review of single-particle Quantum Mechanics

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Topics for Quantum Mechanics II

Single particle analysis
- Single particle interacting with electromagnetic fields – EC Chap. 9
- Scattering of a particle from a spherical potential – EC Chap. 14
- More time independent perturbation methods – EC Chap. 12, 13
- Single electron states of a multi-well potential ➔ molecules and solids – EC Chap. 2,6
- Time dependent perturbation methods – EC Chap. 15
- Relativistic effects and the Dirac Equation – EC Chap. 16
- Path integral formalism (Feynman) – EC Chap. 11.C

Multiple particle analysis
- Quantization of the electromagnetic fields – EC Chap. 17
- Photons and atoms – EC Chap. 18
- Multi particle systems; Bose and Fermi particles – EC Chap. 10
- Multi electron atoms and materials
  - Hartree-Fock approximation
  - Density functional approximation

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Comment on exam

Three multipart problems

Be careful about units. Professor Carlson's text is in SI units. Many graduate level texts are in cgs Gaussian units as are some of the PHY 742 lecture notes. It is often convenient/advisable to convert to dimensionless units.

In your spare time, think about your presentation topic

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Interaction of a particle of mass *m* and charge *q* with an electromagnetic field:

Classical Hamiltonian in SI units:

$$H(\mathbf{r},\mathbf{p},t)=\frac{1}{2m}\left(\mathbf{p}-q\mathbf{A}(\mathbf{r},t)\right)^2+V(\mathbf{r})+qU(\mathbf{r},t)$$

Quantum Hamiltonian in SI units and in coordinate representation:

$$\mathbf{p}\rightarrow -i\hbar\nabla$$

$$H(\mathbf{r},t)=\frac{1}{2m}\left(-i\hbar\nabla-q\mathbf{A}(\mathbf{r},t)\right)^2+V(\mathbf{r})+qU(\mathbf{r},t)$$

Note: In EC's text, $q\leftrightarrow -e$

Relationship of scalar and vector potentials to electric and magnetic fields:

Electric field: $\mathbf{E}(\mathbf{r},t)=-\frac{\partial\mathbf{A}(\mathbf{r},t)}{\partial t}-\nabla U(\mathbf{r},t)$

Magnetic field: $\mathbf{B}(\mathbf{r},t)=\nabla\times\mathbf{A}(\mathbf{r},t)$

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Summary of results --

Schrödinger equation:

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}=H(\mathbf{r},t)\Psi(\mathbf{r},t)$$

$$H(\mathbf{r},t)=\frac{1}{2m}\left(-i\hbar\nabla-q\mathbf{A}(\mathbf{r},t)\right)^2+V(\mathbf{r})+qU(\mathbf{r},t)$$

Particle charge density: $\rho(\mathbf{r},t)=q\left|\Psi(\mathbf{r},t)\right|^2$

Particle current density $\mathbf{j}$:

$$\mathbf{j}(\mathbf{r},t)=\frac{qi\hbar}{2m}\left(\Psi(\mathbf{r},t)\nabla\Psi^*(\mathbf{r},t)-\Psi^*(\mathbf{r},t)\nabla\Psi(\mathbf{r},t)\right)-\frac{q^2}{m}\mathbf{A}(\mathbf{r},t)\left|\Psi(\mathbf{r},t)\right|^2$$

Continuity equation: $\frac{\partial\rho}{\partial t}+\nabla\cdot\mathbf{j}=0$

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Consideration of effects of a static magnetic field on quantum states of a charged free particle. First consider the spatial degrees of freedom (ignoring intrinsic spin).

Assume particle has charge q and mass m; $V(\mathbf{r})=0$ and $U(\mathbf{r})=0$

$$H=\frac{1}{2m}\left(-i\nabla-q\mathbf{A}(\mathbf{r})\right)^2$$

For a constant and uniform magnetic field $B_0\hat{\mathbf{z}}$

can choose $\mathbf{A}(\mathbf{r})=-B_0 y\hat{\mathbf{x}}$

$$H=\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}+qB_0 y\right)^2+\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)$$

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$$H = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x} + qB_0 y\right)^2 + \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

$$H\Psi = e^{i(p_x x + p_z z)/\hbar}\left(-\frac{\hbar^2}{2m}\frac{d^2\psi(y)}{dy^2} + \left(\frac{1}{2}m\omega_c^2(y-y_0)^2 + \frac{p_z^2}{2m}\right)\psi(y)\right) = E\Psi$$

Differential equation for $\psi(y)$:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(y)}{dy^2} + \frac{1}{2}m\omega_c^2(y-y_0)^2\psi(y) = \left(E - \frac{p_z^2}{2m}\right)\psi(y)$$

where $\omega_c \equiv \frac{qB_0}{m}$ $\quad y_0 = -\frac{p_x}{qB_0}$

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$$-\frac{\hbar^2}{2m}\frac{d^2\psi(y)}{dy^2} + \frac{1}{2}m\omega_c^2(y-y_0)^2\psi(y) = \left(E - \frac{p_z^2}{2m}\right)\psi(y)$$

where $\omega_c \equiv \frac{qB_0}{m}$

Energy eigenvalues:

$$E = E_n(p_z) = \hbar\omega_c\left(n + \frac{1}{2}\right) + \frac{p_z^2}{2m}$$

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Interaction of magnetostatic field B with a hydrogen atom (including contribution of intrinsic electron spin, omitting contribution of intrinsic proton spin).

Isolated H atom: $H^0 = \frac{\mathbf{p}^2}{2m} + V(r)$

H atom in magnetic field **B** and vector potential $\mathbf{A} = -\frac{1}{2}\mathbf{r}\times\mathbf{B}$

$$H = \frac{(\mathbf{p}+e\mathbf{A})^2}{2m} + V(r) + g\mu_B\mathbf{S}\cdot\mathbf{B}/\hbar = H^0 + H^1 + H^2$$

Terms of linear order in **A**:

$$\frac{e}{2m}(\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}) = -\frac{e}{4m}\left(\mathbf{p}\cdot(\mathbf{r}\times\mathbf{B}) + (\mathbf{r}\times\mathbf{B})\cdot\mathbf{p}\right) = \frac{e}{2m}(\mathbf{r}\times\mathbf{p})\cdot\mathbf{B} = \frac{e}{2m}\mathbf{L}\cdot\mathbf{B}$$

$$H^1 = \mu_B(\mathbf{L} + g\mathbf{S})\cdot\mathbf{B}/\hbar$$

$$\mu_B = \frac{e\hbar}{2m} \qquad |g| = 2.00231930436256$$

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Analysis of magnetostatic effects on atomic structure using perturbation theory, also including the effects of spin-orbit interaction

$$H = \frac{(\mathbf{p}+e\mathbf{A})^2}{2m} + V(r) + G(r)\mathbf{S}\cdot\mathbf{L} + g\mu_B\mathbf{B}\cdot\mathbf{S}/\hbar$$

$$H^0 = \frac{\mathbf{p}^2}{2m} + V(r)$$

Keeping terms of linear order in $\mathbf{B}$ and spin-orbit interation :

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

$$H^1 = G(r)\mathbf{S}\cdot\mathbf{L} + \mu_B(\mathbf{L}+g\mathbf{S})\cdot\mathbf{B}/\hbar$$

$$= \frac{G(r)}{2}\left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right) + \mu_B\left(\mathbf{J}+(g-1)\mathbf{S}\right)\cdot\mathbf{B}/\hbar$$

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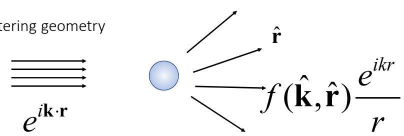
Representation of scattering in terms of probability amplitude

Scattering geometry



Incident plane wave with wavevector $\mathbf{k}$ and energy $E = \frac{\hbar^2 k^2}{2m}$

Scattered spherical wave with scattering amplitude $f(\hat{\mathbf{k}},\hat{\mathbf{r}})$

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What we want to show, is that the scattering phase shift is a measure of the quantum mechanical scattering cross section:

Differential scattering cross section

$$\frac{d\sigma}{d\Omega} = \frac{\text{Probability of particle scattering}}{\text{Incident flux of particles}}$$

$$= \left|f(\hat{\mathbf{k}},\hat{\mathbf{r}})\right|^2$$

$$= \left(\frac{4\pi}{k}\right)^2 \left|\sum_{lm} e^{i\delta_l(E)}\sin(\delta_l(E))Y^*_{lm}(\hat{\mathbf{k}})Y_{lm}(\hat{\mathbf{r}})\right|^2$$

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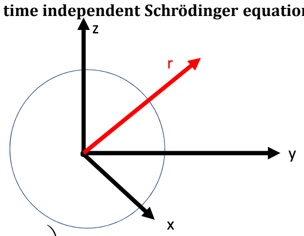
Representation of a free particle in quantum mechanics --

Continuum solutions of the time independent Schrödinger equation.



$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\Psi_E(\mathbf{r}) = E\Psi_E(\mathbf{r})$$

Potential interaction due to spherical target for $0 \leq r \leq D$

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If the system has spherical symmetry about a given origin, it is then convenient to expand the eigenfunctions into spherical harmonic functions:

$$\Psi_E(\mathbf{r}) = \sum_{lm} R_{El}(r) Y_{lm}(\hat{\mathbf{r}})$$

Differential equation for radial function

$$\left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}\right) + V(r) - E\right) R_{El}(r) = 0$$

For many cases, $V(r \to \infty) \approx 0$

In the range that $V(r)$ sufficiently small, the radial equation satisfies:

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + \frac{2mE}{\hbar^2}\right) R^0_{El}(r) = 0 \qquad \text{for } E > 0$$

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In the range for $V(r) \approx 0$:

$$R_{El}(r) = A_l j_l(kr) + B_l y_l(kr) = \mathcal{N}\left(\cos\delta_l j_l(kr) - \sin\delta_l y_l(kr)\right)$$

Note that if $V(r) \equiv 0$, we expect $\delta_l = 0$.

How to determine phase shifts $\delta_l(E)$:

Suppose the range of the scattering potential is D:

For $r < D$, solve differential equation:

$$\left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}\right) + V(r) - E\right) R_{El}(r) = 0$$

Continuity conditions at $r = D$:

Note that in Professor Carlson's text: $y_l(z) \Leftrightarrow n_l(z)$

$$R_{El}(D) = \mathcal{N}\left(\cos\delta_l j_l(kD) - \sin\delta_l y_l(kD)\right)$$

$$\frac{dR_{El}(D)}{dr} = \mathcal{N}\left(\cos\delta_l \frac{dj_l(kD)}{dr} - \sin\delta_l \frac{dy_l(kD)}{dr}\right)$$

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Continuity conditions at $r = D$ -- continued:

$$R_{El}(D) = \mathcal{N}\left(\cos\delta_l\, j_l(kD) - \sin\delta_l\, y_l(kD)\right)$$

$$\frac{dR_{El}(D)}{dr} = \mathcal{N}\left(\cos\delta_l \frac{dj_l(kD)}{dr} - \sin\delta_l \frac{dy_l(kD)}{dr}\right)$$

Some identities:

$$j_l(z)\frac{dy_l(z)}{dz} - y_l(z)\frac{dj_l(z)}{dz} = \frac{1}{z^2}$$

$$\frac{d\ln\left(R_{El}(r)\right)}{dr} = \left.\frac{\frac{dR_{El}(r)}{dr}}{R_{El}(r)}\right|_{r=D} \equiv L_l(E)$$

$$\tan\delta_l(E) = \frac{L_l(E)\, j_l(kD) - k j_l'(kD)}{L_l(E)\, y_l(kD) - k y_l'(kD)}$$

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Variational methods --

Significance of this inequality -- $$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0$$

The inequality motivates a class of estimation methods known as variational methods to converge to the ground state energy E_0 and the corresponding ground state probability amplitude.

Define $$E_{trial}(\Psi_{trial}) \equiv \frac{\langle\psi_{trial}|H|\psi_{trial}\rangle}{\langle\psi_{trial}|\psi_{trial}\rangle}$$

Minimize $E_{trial}(\Psi_{trial})$ with respect to Ψ_{trial}

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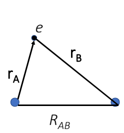
Quantum states of H_2^+



$$r_A \equiv r$$
$$r_B \equiv |\mathbf{r} - \mathbf{R}|$$
$$\mathbf{R}_{AB} \equiv \mathbf{R} = R\hat{\mathbf{z}}$$

Assuming that the nuclear positions are fixed:
Schrödinger equation for electron

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r} - \frac{e^2}{|\mathbf{r}-\mathbf{R}|} + \frac{e^2}{R}$$

$$H\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

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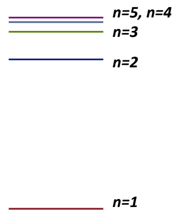
Recall the eigenstates of a H atom --



$$H_{atom} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r}$$

$$H_{atom}\psi_{atom}(\mathbf{r}) = E_{atom}\psi_{atom}(\mathbf{r})$$

$$\psi_{atom}(\mathbf{r}) \rightarrow \psi_{nlm}(\mathbf{r}) = R_{nl}(r)Y_{lm}(\hat{\mathbf{r}})$$

$$E_{atom} \rightarrow E_n = -\frac{e^2}{2a_0 n^2} \qquad n = 1,2,3....$$

$$\psi_{100}(r) = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}$$

Useful basis for representing states of H_2^+ ion

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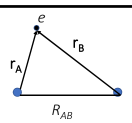

Trial wavefunction:

$$\Psi(\mathbf{r}) = C_A\psi(r_A) + C_B\psi(r_B)$$

where $\psi(r) = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}$

Note that: $\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r}\right)\psi(r) = \varepsilon_{1s}\psi(r)$

$$\varepsilon_{1s} = -\frac{e^2}{2a_0}$$

Variational estimate of coefficients C_A and C_B :

$$U(C_A, C_B) = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

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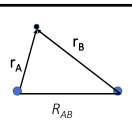

$$\langle\Psi|\Psi\rangle = C_A^2 + C_B^2 + 2C_A C_B \Delta$$

where $\Delta \equiv \int d^3r\ \psi(r_A)\ \psi(r_B) = e^{-D}\left(1 + D + \frac{1}{3}D^2\right)$

$$D = R_{AB}/a_0 \equiv R/a_0$$

Some details: Let $s \equiv r/a_0$

$$\int d^3r\ \psi(r_A)\ \psi(r_B) = \frac{2\pi}{\pi}\int_{-1}^{1} dx \int_0^\infty s^2 ds\ e^{-s} e^{-\sqrt{s^2+D^2-2sDx}}$$

$$= 2\int_0^\infty s^2 ds e^{-s} \int_{s+D}^{|s-D|} \frac{udu}{sD} e^{-u} = e^{-D}\left(1 + D + \frac{D^2}{3}\right)$$

$$\langle\Psi|H|\Psi\rangle = C_A^2 H_{AA} + C_B^2 H_{BB} + 2C_A C_B H_{AB}$$

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Optimization wrt coefficients C_A and C_B :

$$U(C_A,C_B)=\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}=\frac{C_A^2H_{AA}+C_B^2H_{BB}+2C_AC_BH_{AB}}{C_A^2+C_B^2+2C_AC_B\Delta}$$

Constraint: $\langle\Psi|\Psi\rangle=C_A^2+C_B^2+2C_AC_B\Delta=1$

$$\min\left(U(C_A,C_B)\right)\quad\Rightarrow\begin{pmatrix}H_{AA}&H_{AB}\\H_{AB}&H_{BB}\end{pmatrix}\begin{pmatrix}C_A\\C_B\end{pmatrix}=U\begin{pmatrix}1&\Delta\\\Delta&1\end{pmatrix}\begin{pmatrix}C_A\\C_B\end{pmatrix}$$

Two solutions:

$$U_+=\frac{H_{AA}+H_{AB}}{1+\Delta}\qquad\Psi_+(r)=\sqrt{\frac{1}{2(1+\Delta)}}\left(\psi(r_A)+\psi(r_B)\right)$$

$$U_-=\frac{H_{AA}-H_{AB}}{1-\Delta}\qquad\Psi_-(r)=\sqrt{\frac{1}{2(1-\Delta)}}\left(\psi(r_A)-\psi(r_B)\right)$$

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Evaluation of matrix elements:

$$H=-\frac{\hbar^2}{2m}\nabla^2-\frac{e^2}{r}-\frac{e^2}{|\mathbf{r}-\mathbf{R}|}+\frac{e^2}{R}$$

$$H_{AA}=H_{BB}=\langle\psi(r)|H|\psi(r)\rangle$$

$$=\frac{e^2}{2a_0}\left(-1+\frac{2}{D}-\frac{2}{D}+2e^{-2D}\left(1+\frac{1}{D}\right)\right)$$

Note that:

$$\langle\psi(r)|-\frac{e^2}{|\mathbf{r}-\mathbf{R}|}|\psi(r)\rangle=-\frac{4e^2}{a_0}\int_0^\infty s^2ds\frac{1}{s_>}e^{-2s}$$

$$=-\frac{e^2}{a_0D}\left(1-e^{-2D}\left(D+1\right)\right)$$

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Evaluation of matrix elements – summary --

$$H=-\frac{\hbar^2}{2m}\nabla^2-\frac{e^2}{r}-\frac{e^2}{|\mathbf{r}-\mathbf{R}|}+\frac{e^2}{R}$$

$$H_{AA}=H_{BB}=\langle\psi(r)|H|\psi(r)\rangle$$

$$=\frac{e^2}{2a_0}\left(-1+\frac{2}{D}-\frac{2}{D}+2e^{-2D}\left(1+\frac{1}{D}\right)\right)$$

$$H_{AB}=H_{BA}=\langle\psi(r)|H|\psi\left(|\mathbf{r}-\mathbf{R}|\right)\rangle$$

$$=\frac{e^2}{2a_0}\left(\left(-1+\frac{2}{D}\right)\Delta-2e^{-D}\left(1+D\right)\right)$$

$$\langle\psi(r)|\psi\left(|\mathbf{r}-\mathbf{R}|\right)\rangle\equiv\Delta=e^{-D}\left(1+D+\frac{D^2}{3}\right)$$

Two solutions:

$$U_+(D)=\frac{H_{AA}+H_{AB}}{1+\Delta}$$

where $\Psi_+(r)=\sqrt{\frac{1}{2(1+\Delta)}}\left(\psi(r_A)+\psi(r_B)\right)$

$$U_-(D)=\frac{H_{AA}-H_{AB}}{1-\Delta}$$

where $\Psi_-(r)=\sqrt{\frac{1}{2(1-\Delta)}}\left(\psi(r_A)-\psi(r_B)\right)$

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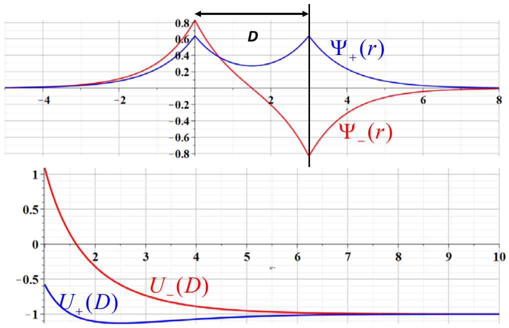

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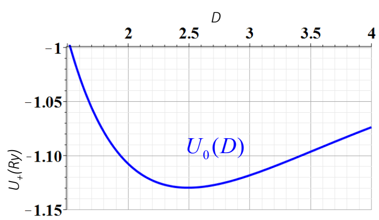

Experimental bond length according to NIST:
~ 2 Bohr

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Fermi Golden Rule

Resonant transition rate due to time harmonic perturbation --

$$\mathcal{R}_{I\to f} = \frac{\left|k^1_{I\to f}(t)\right|^2}{T} \approx \frac{2\pi}{\hbar}\left|\langle f^0|\tilde{H}^1|I^0\rangle\right|^2 \left(\delta\left(\hbar\omega + E_f^0 - E_I^0\right) + \delta\left(-\hbar\omega + E_f^0 - E_I^0\right)\right)$$

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Example – Zero order system in the presence of an electromagnetic field -- continued

Suppose the charged particle is an electron: $q=-e$

$\tilde{H}^1 = eF_0 z$ representing field as scalar potential

$\tilde{H}'^1 = -\frac{eF_0 p_z}{\omega m}$ representing field as vector potential

Note that these two are equivalent in the exact basis of H^0 :

$$\frac{p_z}{m} = \frac{1}{i\hbar}\left[z, \frac{\mathbf{p}^2}{2m}\right] = \frac{1}{i\hbar}\left[z, H^0\right]$$

$$\left\langle f^0 \left| \frac{p_z}{m} \right| I^0 \right\rangle = \frac{1}{i\hbar}\left\langle f^0 \left| \left[z, H^0\right] \right| I^0 \right\rangle = -\frac{E_f^0 - E_I^0}{i\hbar}\left\langle f^0 \left| z \right| I^0 \right\rangle$$

$$= i\omega_{fI}\left\langle f^0 \left| z \right| I^0 \right\rangle \quad \text{for } \hbar\omega_{fI} \equiv E_f^0 - E_I^0$$

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Dirac equation for electron in the field of a H-like ion

$$H = \begin{pmatrix} mc^2 + V(r) & \mathbf{p}\cdot\boldsymbol{\sigma}c \\ \mathbf{p}\cdot\boldsymbol{\sigma}c & -mc^2 + V(r) \end{pmatrix}$$

Note that the following operators commute with the Hamiltonian and have simultaneous eigenvalues:

$$J_z = \begin{pmatrix} L_z + \frac{1}{2}\hbar\sigma_z & 0 \\ 0 & L_z + \frac{1}{2}\hbar\sigma_z \end{pmatrix}$$

$$\mathbf{J}^2 = \begin{pmatrix} \mathbf{L}^2 + \frac{3\hbar^2}{4}I_2 + \hbar\boldsymbol{\sigma}\cdot\mathbf{L} & 0 \\ 0 & \mathbf{L}^2 + \frac{3\hbar^2}{4}I_2 + \hbar\boldsymbol{\sigma}\cdot\mathbf{L} \end{pmatrix}$$

$$K = \begin{pmatrix} \boldsymbol{\sigma}\cdot\mathbf{L} + \hbar I_2 & 0 \\ 0 & -\boldsymbol{\sigma}\cdot\mathbf{L} - \hbar I_2 \end{pmatrix}$$

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Further consideration of the full Hamiltonian:

$$H = \begin{pmatrix} mc^2 + V(r) & (\hat{\mathbf{r}}\cdot\boldsymbol{\sigma})^2(\mathbf{p}\cdot\boldsymbol{\sigma})c \\ (\hat{\mathbf{r}}\cdot\boldsymbol{\sigma})^2(\mathbf{p}\cdot\boldsymbol{\sigma})c & -mc^2 + V(r) \end{pmatrix}$$

$$= \begin{pmatrix} mc^2 + V(r) & (\hat{\mathbf{r}}\cdot\boldsymbol{\sigma})(\hat{\mathbf{r}}\cdot\mathbf{p} + i\boldsymbol{\sigma}\cdot\mathbf{L}/r)c \\ (\hat{\mathbf{r}}\cdot\boldsymbol{\sigma})(\hat{\mathbf{r}}\cdot\mathbf{p} + i\boldsymbol{\sigma}\cdot\mathbf{L}/r)c & -mc^2 + V(r) \end{pmatrix}$$

Eigenvalue problem:

$$H\begin{pmatrix} g_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}}) \\ if_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}}) \end{pmatrix} = E\begin{pmatrix} g_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}}) \\ if_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}}) \end{pmatrix}$$

Coupled differential equations for radial functions:

$$\left(V(r) + mc^2 - E\right)g_{E\kappa J}(r) = \hbar c\left(\frac{d}{dr} + \frac{-\kappa + 1}{r}\right)f_{E\kappa J}(r)$$

$$\left(V(r) - mc^2 - E\right)f_{E\kappa J}(r) = -\hbar c\left(\frac{d}{dr} + \frac{\kappa + 1}{r}\right)g_{E\kappa J}(r)$$

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cgs Gaussian units

For $V(r) = \frac{Ze^2}{r}$

$$\alpha = \frac{e^2}{\hbar c} = \frac{1}{\mathbf{137.035999084}}$$

SI units

For $V(r) = \frac{Ze^2}{4\pi\epsilon_0 r}$

$$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} = \frac{1}{\mathbf{137.035999084}}$$

Exact solution of Dirac equation for H-like ion:

$$E_n = \frac{mc^2}{\left(1 + \frac{Z^2\alpha^2}{\left(\left((J+\frac{1}{2})^2 - Z^2\alpha^2\right)^{1/2} - (J+\frac{1}{2}) + n\right)^2}\right)^{1/2}}$$

for $n = (J+\frac{1}{2}), (J+\frac{1}{2}+1), (J+\frac{1}{2}+2), \ldots$

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