FI 002 – Mecânica Quântica II – Lista 3

P.01. P.11.7, Baym:
Estimate the ground state energy of the hydrogen atom using a three-dimensional harmonic oscillator ground state wave function as a trial function.

P.02. P.8.2 and P.8.3, Merzbacher**:
Using scaled variables, as in Section 5.1, consider the anharmonic oscillator Hamiltonian,

$$H = \frac{1}{2}p_\xi^2 + \frac{1}{2}\xi^2 + \lambda\xi^4,$$

where λ is a real-valued parameter.

a) Estimate the ground state energy by a variational calculation using as a trial function the ground state wave function for the harmonic oscillator

$$H_0(\omega) = \frac{1}{2}p_\xi^2 + \frac{1}{2}\omega^2\xi^2,$$

where ω is an adjustable variational parameter. Derive an equation that relates ω and λ.

b) Compute the variational estimate of the ground state energy of H for various positive values of the strength λ.

c) In first-order perturbation theory, calculate the change in the ground-state energy of a linear harmonic oscillator that is perturbed by a potential gx^4,

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 + gq^4 = H_0 + gq^4 = H_0 + V.$$

For small values of the coefficient, compare the result with the variational calculation above.

03. P.8.4, Merzbacher:
Using a Gaussian trial function $e^{-\lambda x^2}$ with an adjustable parameter, make a variational estimate of the ground state energy for a particle in a Gaussian potential well, represented by the Hamiltonian

$$H = \frac{p^2}{2m} - V_0 e^{-\alpha x^2}, \qquad \text{where } V_0 > 0 \text{ and } \alpha > 0.$$

04. P.12.15, Merzbacher:
Apply the variational method to the ground state ($l = 0$) of a particle moving in an attractive (Yukawa or screened Coulomb or Debye) potential

$$V(r) = V_0 \frac{e^{-r/a}}{r/a}, \qquad (V_0 > 0).$$

Use as a trial function

$$R(r) = e^{-\gamma r/a}$$

with an adjustable parameter γ. Obtain the ' 'best" trial wave function of this form and deduce a relation between γ and the strength parameter $2mv_0a^2/\hbar^2$. Evaluate γ and calculate an upper bound to the energy for $2mv_0a^2/\hbar^2 = 2.7$. Show that in the limit of the Coulomb potential ($V_0 \to 0$, $a \to \infty$, $V_0 a$ finite) the correct energy and wave function for the hydrogenic atom are obtained.

P.05. P.19.3 and P.19.4, Desai:

a) Solve the Schrödinger equation in one dimension given by

$$\frac{d^2u}{dx^2} + k^2 u(x) = \frac{2m}{\hbar^2} V(x) u(x)$$

using the Green's function formalism by writing

$$u(x) = u_0(x) + \frac{2m}{\hbar^2} \int dx' G_0(x - x') V(x') u(x').$$

Show that, for the outgoing wave boundary condition, G_0 is given by

$$G_0(x - x') = \begin{cases} -\frac{i}{2k} e^{ik(x-x')}, & x > x' \\ -\frac{i}{2k} e^{-ik(x-x')}, & x < x'. \end{cases}$$

b) Using the Green's function obtained in item (a), determine the wavefunction $u(x)$ for $x > 0$ and $x < 0$ for an attractive delta function potential given by

$$\frac{2m}{\hbar^2} V(x) = -\lambda \delta(x).$$

Also, obtain the reflection R and transmission T coefficients.

c) The one-dimensional δ-function potential with $\lambda > 0$ admits one (and only one) bound state for any value of λ. Show that the transmission and reflection amplitudes you computed have bound-state poles at the expected positions when k is regarded as a complex variable.
Hint: Eq. (6.54), Merzbacher.

d) **Optional:** Similar to item (b), determine the wavefunction $u(x)$ for the potential

$$V(x) = \begin{cases} -V_0, & |x| < a, \\ 0, & |x| > a, \end{cases}$$

where V_0 and a are positive constantes.
Hint: Define $k_0^2 = 2mV_0/\hbar^2$ and Eq. (6.63), Merzbacher.

P.06. P.21.1, Desai:
Consider the elastic scattering from the spherical square well

$$V(r) = \begin{cases} V_0, & 0 < r \leq a, \\ 0, & r > a, \end{cases}$$

where V_0 and a are positive constants, and the energy of the incident particles is $0 < E < V_0$.

a) For the s-wave scattering ($l = 0$), determine the parameters $\beta_l(k)$, $\xi_l(k)$, $\Delta_l(k)$, and $s_l(k)$ (see Sec. 13.6, Merzbacher) and then calculate the s-wave phase shift $\delta_0(k)$.

b) For the p-wave scattering ($l = 1$), determine the parameters $\beta_l(k)$, $\xi_l(k)$, $\Delta_l(k)$, and $s_l(k)$ and then calculate the s-wave phase shift $\delta_1(k)$.

c) For the s-wave scattering, determine the scattering amplitude $f_{0,k}(\theta)$ and the total cross-section σ_0. Plot the phase shift and the total cross section in terms of ka for a fixed value of $k_0 a$, where $\hbar k_0 = \sqrt{2mV_0}$.

d) For the s-wave scattering, determine the behaviour of the total cross section σ_0 in the low-energy limit.

e) For the p-wave scattering, determine the total cross-section σ_1. Plot the phase shift and the total cross section in terms of ka for a fixed value of $k_0 a$.

P.07. P.19.3, Messiah:
Consider the elastic scattering from a 3-D square well of depth V_0 and radius a and determine the differential cross section within the first Born approximation. Find an expression between V_0 and a such that the Born approximation is valid.

P.08. P.19.3, Messiah:
Consider the elastic scattering from the potential

$$V(r) = V_0 \exp(-r/a),$$

where V_0 and a are positive constants, and determine the differential cross section and the total cross section within the first Born approximation. Find an expression between V_0 and a such that the Born approximation is valid.

09. P.19.3, Messiah:
Consider the elastic scattering from the Gaussian potential

$$V(r) = V_0 \exp(-r^2/a^2),$$

where V_0 and a are positive constants, and determine the differential cross section and the total cross section within the first Born approximation. Find an expression between V_0 and a such that the Born approximation is valid.

10. P.19.3, Messiah:
Consider the elastic scattering from the Yukawa potential

$$V(r) = V_0 \frac{1}{\alpha r} \exp(-\alpha r),$$

where V_0 and α are positive constants, and determine the differential cross section and the total cross section within the first Born approximation. Find an expression between V_0 and α such that the Born approximation is valid.

11. Ex. 13.16, Merzbacher:
Consider the elastic scattering from the spherical square well

$$V(r) = \begin{cases} -V_0, & 0 < r \le a, \\ 0, & r > a, \end{cases}$$

where V_0 and a are positive constants.

a) For the s-wave scattering ($l = 0$), determine the parameters $\beta_l(k)$, $\xi_l(k)$, $\Delta_l(k)$, and $s_l(k)$ (see Sec. 13.6, Merzbacher) and then calculate the s-wave phase shift $\delta_0(k)$.

b) For the p-wave scattering ($l = 1$), determine the parameters $\beta_l(k)$, $\xi_l(k)$, $\Delta_l(k)$, and $s_l(k)$ and then calculate the s-wave phase shift $\delta_1(k)$.

c) For the s-wave scattering, determine the scattering amplitude $f_{0,k}(\theta)$ and the total cross-section σ_0. Plot the phase shift and the total cross section in terms of ka for a fixed value of $k_0 a$, where $\hbar k_0 = \sqrt{2mV_0}$.

d) For the s-wave scattering, determine the behaviour of the total cross section σ_0 in the low-energy limit.

e) For the p-wave scattering, determine the total cross-section σ_1. Plot the phase shift and the total cross section in terms of ka for a fixed value of $k_0 a$.

P.12. Ex.4.14, Ex.13.7 and P.13.2, Merzbacher**:
Consider that the scattering potential has the translation invariance property $V(\mathbf{r}+\mathbf{R}) = V(\mathbf{r})$, where $\mathbf{R}$ is a constant vector.

a) If $\mathbf{d}_1$, $\mathbf{d}_2$, and $\mathbf{d}_3$ are the primitive translation vectors of a three-dimensional infinite lattice whose points are at positions $\mathbf{R} = n_1\mathbf{d}_1 + n_2\mathbf{d}_2 + n_3\mathbf{d}_3$ (n_i integer), show that any simultaneous eigenfunction of all the translation operators $D(\mathbf{R}) = e^{-i\mathbf{k}\cdot\mathbf{R}}$ corresponding to eigenvalues $e^{-i\mathbf{k}\cdot\mathbf{R}}$ is of the form $u(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}$, where $u(\mathbf{r})$ is an arbitrary periodic function of $\mathbf{r}$ over the lattice, i.e., $u(\mathbf{r}+\mathbf{R}) = u(\mathbf{r})$, for every $\mathbf{R}$. Note that any two values of $\mathbf{k}$ which produce the same eigenvalue $e^{-i\mathbf{k}\cdot\mathbf{R}}$ differ by a a reciprocal lattice vector $\mathbf{G}$, defined by the condition $\mathbf{G}\cdot\mathbf{R} = 2n\pi$, where n is any integer.

b) Show that in the first Born approximation, as in the exact formulation below, scattering occurs only when the momentum transfer $\mathbf{q}$ (in units of $\hbar$) equals a reciprocal lattice vector $\mathbf{G}$.

c) Prove that the scattering solutions $\psi^{(\pm)}_{\mathbf{k}}(\mathbf{r})$ of the integral form of the Schrödinger equation are Bloch wave functions, since they satisfy the relation

$$\psi^{(\pm)}_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi^{(\pm)}_{\mathbf{k}}(\mathbf{r}).$$

d) Show that the scattering amplitude vanishes unless $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ is a reciprocal lattice vector (Exercise 4.14) which satisfies the condition

$$\mathbf{q}\cdot\mathbf{R} = (\mathbf{k}-\mathbf{k}')\cdot\mathbf{R} = 2n\pi,$$

where n is an integer. This relation is the Laue condition familiar in condensed matter physics.

P.13. P.20.4, Merzbacher:
Using the Bom approximation, and neglecting relativistic effects, express the differential cross section for scattering of an electron from a spherically symmetric charge distribution $\rho(r)$ as the product of the Rutherford scattering cross section for a point charge and the square of a form factor $F(q)$,

$$\frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left(\frac{4\pi}{q^2}\right)^2 F^2(q),$$

where $\mathbf{q}$ is the transfer momentum. Obtain an expression for the form factor $F(q)$ and then evaluate it as a function of the momentum transfer for

a) a uniform charge distribution of radius R;

b) a Gaussian charge distribution with the same root-mean-square radius.

Hint.: Starting point: Eq. (13.49), Merzbacher. See also P.20.2, Merzbacher.

14. P.20.1, Merzbacher:
Obtain the "scattering states" (energy eigenstates with $E \geq 0$) for a one-dimensional delta-function potential, $\delta(x)$. Calculate the matrix elements $\langle k'|S|k\rangle$ and verify the unitarity of the S matrix. Obtain the transmission coefficient, and compare with Eq. (6.19) and Exercise 6.13. Perform the calculations in both the coordinate and momentum representations.

15. P.20.2, Merzbacher:
Use the Bom approximation to calculate the differential and total cross sections for the elastic scattering of electrons by a hydrogen atom that is in its ground state. Approximate the interaction between the continuum electron and the atom by the static field of the atom and neglect exchange phenomena.

P.16. P.20.5, Merzbacher:
If the nonlocal *separable* scattering potential

$$\langle \mathbf{r}'|V|\mathbf{r}\rangle = \lambda u(r')u(r)$$

is given, work out explicitly and solve the integral equation for $\psi_{\mathbf{k}}^{(+)}(\mathbf{r})$. Obtain the scattering amplitude and discuss the Born series for this potential.
Hint: Eq. Lippmann-Schwinger and T-matrix. See also Sec.8.2.b, Gottfried.

17. Ex.20.7, Merzbacher:
Transform the matrix element (20.79),

$$\langle \mathbf{k}'|S|\mathbf{k}\rangle = \delta(k-k')\sum_{l=0}^{\infty}\frac{2l+1}{4\pi k^2}e^{2i\delta_l(k)}P_l\left(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}'\right)$$

into the orbital angular momentum representation (see Exercise 17.40), and show that (modified)

$$\langle \alpha\, l'\, m'|S|\alpha\, l\, m\rangle = \delta_{m',m}\delta_{l',l}\int dk\, k^2|R_\alpha(k)|^2 e^{2i\delta_l(k)}$$

verifying that $e^{2i\delta_l(k)}$ are the eigenvalues of the S matrix for a rotationally invariant interaction, in agreement with Eq. (13.75).

18. Ex.20.9, Merzbacher:
Show that the first Bom approximation violates the optical theorem. Explain this failure and show how it can be remedied by including the second Born approximation for the forward scattering amplitude.

P.19. P.6.10, Sakurai:
Consider the s-wave ($l = 0$) elastic scattering from a repulsive spherical delta potential

$$\frac{2m}{\hbar^2} V(r) = \gamma \delta(r - a),$$

where a and γ are positive constants.

a) Show that the s-wave phase shift $\delta_0(k)$ is given by

$$\delta_0(k) = -ka + \tan^{-1}\left(\frac{ka \tan ka}{ka + \gamma a \tan ka}\right),$$

where $\hbar^2 k^2 = 2mE$.
Hint: Follow the procedure described in item (b), P.10.3.b, Cohen.

b) Consider the incident particles in the low-energy limit and determine the differential cross section. Moreover, show that the total cross section reads

$$\sigma_0 = 4\pi a^2 \frac{1}{(ka)^2 + (1 + \gamma a)^2}.$$

P.20. P.6.10, Sakurai:
Consider the s-wave ($l = 0$) elastic scattering from a repulsive spherical delta potential

$$\frac{2m}{\hbar^2} V(r) = \gamma \delta(r - a),$$

where a and γ are positive constants.

a) Show that the s-wave phase shift $\delta_0(k)$ derived in item (a) from the previous problema can be written as

$$\cot \delta_0(k) = -\frac{ka + \gamma a \tan ka + ka \tan^2(ka)}{\gamma a \tan^2(ka)}.$$

b) Plot $\delta_0(ka)$ and $\delta_0(ka) + \pi$ for a fixed value of γa and identify a resonance for $ka \approx \pi$. Recall that it is also possible to identify a resonance via the behaviour of the total cross section σ_0 in terms of ka.

c) Consider that $\gamma a \gg 1$ and $\gamma \gg k$ and show that, up to order $1/\gamma$, the position of the resonance is at $ka \approx \pi\,(1 - 1/\gamma)$. Recall that $\cot \delta_0(k) = 0$ at the position of the resonance.
Hint: Write $ka = \pi + z$ with $|z| \ll 1$.

d) **Optional:** Determine an approximate expression for the resonance width

$$\Gamma = \frac{-2}{(d(\cot \delta_0)/dE)_{E=E_R}}$$

and notice, in particular, that the resonances become extremely sharp as γ becomes large.

P.21. P.10.3.b, Cohen:
Consider a central potential

$$V(r) = \begin{cases} -V_0, & 0 < r \leq a, \\ 0, & r > a, \end{cases}$$

where a and V_0 are positive constant. Set $\hbar k_0^2 = 2mV_0$. We shall confine ourselves to the study of the s-wave ($l = 0$).

a) Bound states $E < 0$. Write the radial equation in the two regions $0 < r \leq a$ and $r > a$ and consider the condition at the origin. Show that, if one sets

$$\rho = \sqrt{\frac{-2mE}{\hbar^2}} \qquad \text{and} \qquad K = \sqrt{k_0^2 - \rho^2},$$

then the radial function $u_0(r)$ is necessarily of the form

$$u_0(r) = \begin{cases} A\exp(-\rho r), & r > a \\ B\sin Kr, & 0 < r \leq a. \end{cases}$$

Write the matching conditions at $r = a$. Deduce from them that the only possible values for ρ are those which satisfy the equation $\rho \tan Ka = -K$.
Plot the above equation as a function of ρa for fixed values of $k_0 a$. Indicate the number of s-bound states as a function of the depth of the well (for fixed R) and show, in particular, that there are no bound states if this depth is too small.
Hint: Eq. (12.7), Merzbacher.
Recall: P.12.1, Merzbacher.

b) Scattering resonances $E > 0$. Again write the radial equation, this time setting

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad \text{and} \qquad K' = \sqrt{k_0^2 + k^2}.$$

Show that the radial function $u_{k,0}(r)$ is of the form

$$u_0(r) = \begin{cases} A\sin(kr + \delta_0), & r > a \\ B\sin K'r, & 0 < r \leq a. \end{cases}$$

Using the continuity conditions at $r = R$, show that the s-wave phase shift $\delta_0(k)$ reads

$$\delta_0(k) = -ka + \tan^{-1}\left(\frac{ka}{K'a}\tan K'a\right).$$

Determine the differential and total cross sections. Plot σ_0 em terms of ka for fixed values of $k_0 a$.

22. P.9.2, Baym:
Consider an experiment in which slow neutrons of momentum $\hbar k$ are scattered by a diatomic molecule; suppose that the molecule is aligned along the y axis with one atom at $y = -b$ and the other at $y = +b$, and that the neutrons are directed along z. Assume the atoms to be infinitely heavy so that they remain fixed throughout the experiment. The potential seen by the neutron from each atom can be adequately represented by a delta function; thus

$$V(r) = a\delta(y-b)\delta(x)\delta(z) + a\delta(y+b)\delta(x)\delta(z).$$

Calculate the scattering amplitude and differential cross section in the Born approximation.

23. P.8.3, Gottfried:
As a 3-D analogue of the 1-D potentials studied in Sec. 4.4(c), consider

$$\frac{2m}{\hbar^2}V(r) = -\lambda\delta(r-a),$$

where λ is a strength parameter having the dimension (length)$^{-1}$.

a) Show that the partial wave scattering amplitude is

$$\frac{1}{\xi}e^{i\delta_i(k)}\sin\delta_l(k) = \frac{gj_i^2(\xi)}{1 - i\xi g j_l(\xi)h_l(\xi)},$$

where $\xi = ka$ and $g = a\lambda$.
Hint: See identity, P.11.7.6, Arfken.

b) Show that the minimum strength required to bind a state of angular momentum l is $g = 2l+1$. In the case of $l = 0$, show that the binding energies $-\eta^2/2ma^2$ are determined by the roots η_n of $2\eta = g(1-e^{-2\eta})$, and that there is just one root if $g > 1$.
Hint.: See item (c), P.6.1, Sakurai.