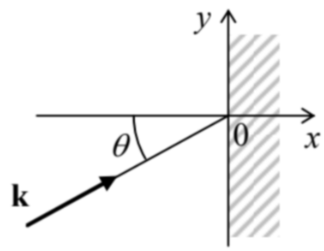
LibreTexts

3.9: Exercise Problems

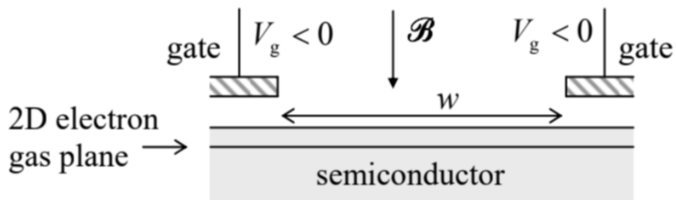
3.1. A particle of energy E is incident (in the figure on the right, within the plane of the drawing) on a sharp potential step:

$$U(\mathbf{r}) = \begin{cases} 0, \text{ for } x < 0, \\ U_0, \text{ for } 0 < x. \end{cases}$$

Calculate the particle reflection probability $\mathscr{R}$ as a function of the incidence angle θ, sketch and discuss this function for various magnitudes and signs of U_0.



3.2. Analyze how are the Landau levels (50) modified by an additional uniform electric field $\mathscr{E}$ directed along the plane of the particle's motion. Contemplate the physical meaning of your result and its implications for the quantum



Hall effect in a gate-defined Hall bar. (The area $l \times w$ of such a bar [see Fig. 6] is defined by metallic gate electrodes parallel to the 2D electron gas plane - see the figure on the right. The negative voltage V_{g}, applied to the gates, squeezes the $2\mathrm{D}$ gas from the area under them into the complementary, Hall-bar part of the plane.)

3.3. Analyze how are the Landau levels (50) modified if a $2\mathrm{D}$ particle is confined in an additional 1D potential well $U(x) = m\omega_0^2 x^2/2$.

3.4. Find the stationary states of a spinless, charged 3D particle moving in "crossed" (mutually perpendicular), uniform electric and magnetic fields, with $\mathscr{E} << \mathscr{B}$. For such states, calculate the expectation values of the particle's velocity in the direction perpendicular to both fields, and compare the result with the solution of the corresponding classical problem.

Hint: You may like to generalize Landau's solution for 2D particles, discussed in Sec. 2.

3.5. Use the Born approximation to calculate the angular dependence and the total cross-section of scattering of an incident plane wave propagating along the x-axis, by the following pair of similar point inhomogeneities:

$$U(\mathbf{r}) = w\left[\delta\left(\mathbf{r} - \mathbf{n}_z \frac{a}{2}\right) + \delta\left(\mathbf{r} + \mathbf{n}_z \frac{a}{2}\right)\right]. \tag{3.9.1}$$

Analyze the results in detail. Derive the condition of the Born approximation's validity for such deltafunctional scatterers.

3.6. Complete the analysis of the Born scattering by a uniform spherical potential (97), started in Sec. 3, by calculation of its total cross-section. Analyze the result in the limits $kR << 1$ and $kR >> 1$.

3.7. Use the Born approximation to calculate the differential cross-section of particle scattering by a very thin spherical shell, whose potential may be approximated as

$$U(r) = w\delta(r - R). \tag{3.9.2}$$

Analyze the results in the limits $kR << 1$ and $kR \gg 1$, and compare them with those for a uniform sphere considered in Sec. 3 .

3.8. Use the Born approximation to calculate the differential and total cross-sections of electron scattering by a screened Coulomb field of a point charge Ze, with the electrostatic potential

$$\phi(\mathbf{r})=\frac{Ze}{4\pi\varepsilon_0 r}e^{-\lambda r}, \tag{3.9.3}$$

neglecting spin interaction effects, and analyze the result's dependence on the screening parameter λ. Compare the results with those given by the classical ("Rutherford") formula [97] for the unscreened Coulomb potential $(\lambda\to 0)$, and formulate the condition of Born approximation's validity in this limit.

3.9. A quantum particle with electric charge Q is scattered by a localized distributed charge with a spherically-symmetric density $\rho(r)$, and zero total charge. Use the Born approximation to calculate the differential cross-section of the forward scattering (with the scattering angle $\theta=0$), and evaluate it for the scattering of electrons by a hydrogen atom in its ground state.

3.10. Reformulate the Born approximation for the 1D case. Use the result to find the scattering and transfer matrices of a "rectangular" (flat-top) scatterer

$$U(x)=\begin{cases}U_0, & \text{for } |x|<d/2\\ 0, & \text{otherwise}\end{cases} \tag{3.9.4}$$

Compare the results with those of the exact calculations carried out earlier in Chapter 2, and analyze how does their relationship change in the eikonal approximation.

3.11. In the tight-binding approximation, find the lowest stationary states of a particle placed into a system of three similar, weakly coupled potential wells located in the vertices of an equilateral triangle.

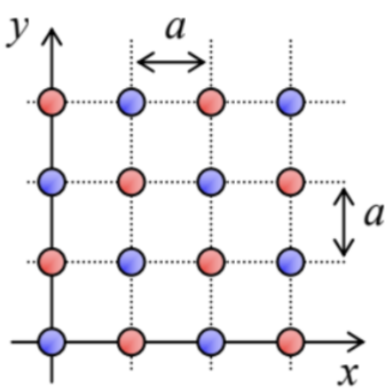
3.12. The figure on the right shows a fragment of a periodic 2D lattice, with the red and blue points showing the positions of different local potentials.

(i) Find the reciprocal lattice and the 1^{st} Brillouin zone of the system.

(ii) Calculate the wave number k of the monochromatic de Broglie wave incident along axis x, at that the lattice creates the lowest-order diffraction peak within the $[x,y]$ plane, and the direction toward this peak.

(iii) Semi-quantitatively, describe the evolution of the intensity of the peak when the local potentials, represented by the different points, become similar.

Hint: The order of diffraction on a multidimensional Bravais lattice is a somewhat ambiguous notion, usually associated with the sum of magnitudes of all integers l_j in Eq. (109), for the vector $\mathbf{Q}$ that is equal to $\mathbf{q}\equiv\mathbf{k}-\mathbf{k}_{\mathrm{i}}$.



3.13. For the 2D hexagonal lattice (Fig. 12b):

(i) find the reciprocal lattice $\mathbf{Q}$ and the 1^{st} Brillouin zone;

(ii) use the tight-binding approximation to calculate the dispersion relation $E(\mathbf{q})$ for a 2D particle moving through a potential profile with such periodicity, with an energy close to the energy of the axially-symmetric states quasi-localized at the potential minima;

(iii) analyze and sketch (or plot) the resulting dispersion relation $E(\mathbf{q})$ inside the 1^{st} Brillouin zone.

3.14. Complete the tight-binding-approximation calculation of the band structure of the honeycomb lattice, started at the end of Sec. 4. Analyze the results; in particular prove that the Dirac points q_{D} are located in the corners of the 1^{st} Brillouin zone, and express the velocity v_n participating in Eq. (122), in terms of the coupling energy δ_n. Show that the final results do not change if the quasilocalized wavefunctions are not axially-symmetric, but are proportional to $\exp\{\mathrm{i}m\varphi\}-$ as they are, with $m=1$, for the $2p_z$ electrons of carbon atoms in graphene, that are responsible for its transport properties.

3.15. Examine basic properties of the so-called Wannier functions defined as

$$\phi_{\mathbf{R}}(\mathbf{r}) \equiv \text{ const } \times \int_{\mathrm{BZ}} \psi_{\mathrm{q}}(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{R}} d^3 q, \tag{3.9.5}$$

where $\psi_{\mathbf{q}}(\mathbf{r})$ is the Bloch wavefunction (108), $\mathbf{R}$ is any vector of the Bravais lattice, and the integration over the quasimomentum $\mathbf{q}$ is extended over any (e.g., the first) Brillouin zone.

3.16. Evaluate the long-range interaction (the so-called London dispersion force) between two similar, electrically-neutral atoms or molecules, modeling each of them as an isotropic 3D harmonic oscillator with the electric dipole moment $\mathbf{d}=q\mathbf{s}$, where $\mathbf{s}$ is the oscillator's displacement from its equilibrium position.

Hint: Represent the total Hamiltonian of the system as a sum of Hamiltonians of independent 1D harmonic oscillators, and calculate their total ground-state energy as a function of the distance between the dipoles. [98]

3.17. Derive expressions for the stationary wavefunctions and the corresponding energies of a $2\mathrm{D}$ particle of mass m, free to move inside a round disk of radius R. What is the degeneracy of each energy level? Calculate the five lowest energy levels with an accuracy better than 1%.

3.18. Calculate the ground-state energy of a $2\mathrm{D}$ particle of mass m, localized in a very shallow flat-bottom potential well

$$U(\rho)=\left\{\begin{array}{r}-U_0, \text{ for } \rho<R, \\ 0, \text{ for } \rho>R,\end{array} \quad \text{with } 0<U_0<<\frac{\hbar^2}{mR^2}.\right.$$

3.19. Estimate the energy E of the localized ground state of a particle of mass m, in an axiallysymmetric 2D potential well of a finite radius R, with an arbitrary but very small potential $U(\rho)$. (Quantify this condition.)

3.20. Spell out the explicit form of the spherical harmonics $Y_4^0(\theta,\varphi)$ and $Y_4^4(\theta,\varphi)$.

3.21. Calculate $\langle x\rangle$ and $\langle x^2\rangle$ in the ground states of the planar and spherical rotators of radius R. What can you say about $\langle p_x\rangle$ and $\langle p_x{}^2\rangle$?

3.22. A spherical rotator, with $r \equiv \left(x^2+y^2+z^2\right)^{1/2}=R=$ const, of mass m is in a state with the following wavefunction: $\psi=\text{const}\times\left(1/3+\sin^2\theta\right)$. Calculate its energy.

3.23. According to the discussion at the beginning of Sec. 5, stationary wavefunctions of a $3\mathrm{D}$ harmonic oscillator may be calculated as products of three 1D "Cartesian oscillators" - see, in particular Eq. (125), with $d=3$. However, according to the discussion in Sec. 6 , the wavefunctions of the type (200), proportional to the spherical harmonics Y_l^m, also describe stationary states of this sphericallysymmetric system. Represent the wavefunctions (200) of:

(i) the ground state of the oscillator, and

(ii) each of its lowest excited states,

as linear combinations of products of $1\mathrm{D}$ oscillator's stationary wavefunctions. Also, calculate the degeneracy of the n^{th} energy level of the oscillator.

3.24. Calculate the smallest depth U_0 of a spherical, flat-bottom potential well

$$U(\mathbf{r})=\left\{\begin{array}{r}-U_0, \text{ for } r<R, \\ 0, \text{ for } R<r,\end{array}\right.$$

at that it has a bound (localized) stationary state. Does such a state exist for a very narrow and deep well $U(\mathbf{r})=-w\delta(\mathbf{r})$, with a positive and finite w ?

3.25. A 3D particle of mass m is placed into a spherically-symmetric potential well with $-\infty<U(r)\leq U(\infty)=0$. Relate its ground-state energy to that of a 1D particle of the same mass, moving in the following potential well:

$$U'(x)=\left\{\begin{array}{ll}U(x), & \text{for } x\geq 0, \\ +\infty, & \text{for } x\leq 0.\end{array}\right. \tag{3.9.6}$$

In the light of the found relation, discuss the origin of the difference between the solutions of the previous problem and Problem 2.17.

3.26. Calculate the smallest value of the parameter U_0, for that the following sphericallysymmetric potential well,

$$U(r)=-U_0 e^{-r/R}, \quad \text{with } U_0, R>0, \tag{3.9.7}$$

has a bound (localized) eigenstate.

Hint: You may like to introduce the following new variables: $f \equiv rR$ and $\xi \equiv Ce^{-r/2R}$, with an appropriate choice of the constant C.

3.27. A particle moving in a certain central potential $U(r)$ has a stationary state with the following wavefunction:

$$\psi=Cr^\alpha e^{-\beta r}\cos\theta, \tag{3.9.8}$$

where C, α, and $\beta>0$ are constants. Calculate:

(i) the probabilities of all possible values of the quantum numbers m and l, and

(ii) the confining potential and the state's energy.

3.28. Use the variational method to estimate the ground-state energy of a particle of mass m, moving in the following spherically-symmetric potential:

$$U(\mathbf{r})=ar^4. \tag{3.9.9}$$

3.29. Use the variational method, with the trial wavefunction $\psi_{\text{trial}}=A/(r+a)^b$, where both $a>0$ and $b>1$ are fitting parameters, to estimate the ground-state energy of the hydrogen-like atom/ion with the nuclear charge $+Ze$. Compare the solution with the exact result. 3.30. Calculate the energy spectrum of a particle moving in a monotonic, but otherwise arbitrary attractive spherically-symmetric potential $U(r)<0$, in the approximation of very large orbital quantum numbers l. Formulate the quantitative condition(s) of validity of your theory. Check that for the Coulomb potential $U(r)=-C/r$, your result agrees with Eq. (201).

Hint: Try to solve Eq. (181) approximately, introducing the same new function, $f(r)\equiv r\mathbb{R}(r)$, that was already used in Sec. 1 and in the solutions of a few earlier problems.

3.31. An electron had been in the ground state of a hydrogen-like atom/ion with nuclear charge Ze, when the charge suddenly changed to $(Z+1)e.99$ Calculate the probabilities for the electron of the changed system to be:

(i) in the ground state, and

(ii) in the lowest excited state.

3.32. Due to a very short pulse of an external force, the nucleus of a hydrogen-like atom/ion, initially at rest in its ground state, starts moving with velocity $\mathbf{v}$. Calculate the probability W_{g} that the atom remains in its ground state. Evaluate the energy to be given, by the pulse, to a hydrogen atom in order to reduce W_{g} to 50%.

3.33. Calculate $\langle x^2\rangle$ and $\langle {p_x}^2\rangle$ in the ground state of a hydrogen-like atom/ion. Compare the results with Heisenberg's uncertainty relation. What do these results tell about the electron's velocity in the system?

3.34. Use the Hellmann-Feynman theorem (see Problem 1.5) to prove:

(i) the first of Eqs. (211), and

(ii) the fact that for a spinless particle in an arbitrary spherically-symmetric attractive potential $U(r)$, the ground state is always an s-state (with the orbital quantum number $l=0$).

3.35. For the ground state of a hydrogen atom, calculate the expectation values of $\mathscr{E}$ and $\mathscr{E}^2$, where $\mathscr{E}$ is the electric field created by the atom, at distances $r \gg r_0$ from its nucleus. Interpret the resulting relation between $\langle \mathscr{O}^2$ and $\langle \mathscr{E}^2\rangle$, at the same observation point.

3.36. Calculate the condition at that a particle of mass m, moving in the field of a very thin spherically-symmetric shell, with

$$U(\mathbf{r})=w\delta(r-R), \tag{3.9.10}$$

and $w<0$, has at least one localized ("bound") stationary state.

3.37. Calculate the lifetime of the lowest metastable state of a particle in the same spherical-shell potential as in the previous problem, but now with $w > 0$, for sufficiently large w. (Quantify this condition.)

3.38. A particle of mass m and energy E is incident on a very thin spherical shell of radius R, whose localized states were the subject of two previous problems, with an arbitrary "weight" w.

(i) Derive general expressions for the differential and total cross-sections of scattering for this geometry.

(ii) Spell out the contribution σ_0 to the total cross-section σ, due to the spherically-symmetric component of the scattered de Broglie wave.

(iii) Analyze the result for σ_0 in the limits of very small and very large magnitudes of w, for both signs of this parameter. In particular, in the limit $w \rightarrow +\infty$, relate the result to the metastable state's lifetime τ calculated in the previous problem.

3.39. Calculate the spherically-symmetric contribution σ_0 to the total cross-section of particle scattering by a uniform sphere of radius R, described by the following potential:

$$U(r)=\begin{cases}U_0, \text{ for } r<R \\ 0, \text{ otherwise}\end{cases}$$

with an arbitrary U_0. Analyze the result in detail, and give an interpretation of its most remarkable features.

3.40. Use the finite difference method with the step $h=a/2$ to calculate as many energy levels as possible, for a particle confined to the interior of:

(i) a square with side a, and

(ii) a cube with side a,

with hard walls. For the square, repeat the calculations, using a finer step: $h=a/3$. Compare the results for different values of h with each other and with the exact formulas.

Hint: It is advisable to either first solve (or review the solution of) the similar 1D Problem 1.15, or start from reading about the finite difference method. [100] Also: try to exploit the symmetry of the systems.

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[97] See, e.g., CM Sec. 3.5, in particular Eq. (3.73).

[98] This explanation of the interaction between electrically-neutral atoms was put forward in 1930 by F. London, on the background of a prior (1928) work by C. Wang. Note that in some texts this interaction is (rather inappropriately) referred to as the "van der Waals force", though it is only one, long-range component of the van der Waals model - see, e.g. SM Sec. 4.1.

[99] Such a fast change happens, for example, at the beta-decay, when one of the nucleus' neurons spontaneously turns into a proton, emitting a high-energy electron and a neutrino, which leave the system very fast (instantly on the atomic time scale), and do not affect directly the atom transition's dynamics.

[100] See, e.g., CM Sec. 8.5 or EM Sec. 2.11.
