Course 624, Quantum Mechanics 2

Mathematical Appendix 3

Radial wave functions in a potential field and phase shifts

a) *Radial Schrödinger equation and integral equation.*

The radial Schrödinger equation (RSE) for the wave function $R_l(r)$ corresponding to the total orbital moment l and energy E reads:

$$\frac{d^2R_l}{dr^2}+\frac{2}{r}\frac{dR_l}{dr}+\left(k^2-\frac{l(l+1)}{r^2}-v(r)\right)R_l=0, \tag{1}$$

where $k^2=2mE/\hbar^2$ and $v(r)=2mV(r)/\hbar^2$. It has two independent solutions, one of which is regular and behaves as r^l at $r\to 0$, whereas the second is singular and behaves as r^{-l-1}. Further we will consider only the regular solution. At $r\to\infty$ this solution asymptotically behaves as:

$$R_l(r)\sim\frac{\sin\left(kr-\frac{l\pi}{2}+\delta_l\right)}{r} \tag{2}$$

The last equation serves as the definition of the phase shift δ_l which is completely due to the potential and is zero for a free partilce. To study the properties of the phase shift, i.e. its dependence on potential, energy and orbitel moment, it is convenient to transform the RSE (1) into an integral equation. Let us transfer the term $v(r)R_l$ to the r.-h-. side of equation and consider it formally as a source term (inhomogeneity) for a free particle RSE with a source:

$$\frac{d^2R_l}{dr^2}+\frac{2}{r}\frac{dR_l}{dr}+\left(k^2-\frac{l(l+1)}{r^2}\right)R_l=q(r)\,;\;q(r)=v(r)R_l \tag{3}$$

The general solution of eq. (3) can be obtained by using the Green function of the homogeneous RSE for a free particle (FRSE) as follows:

$$R_l(r)=R_l^{(0)}(r)+\int_0^\infty G_l(r,r')\,q(r')\,r'^2dr', \tag{4}$$

where $R_l^{(0)}(r)$ is the general solution of the FRSE and $G_l(r,r')$ is the Green function obeying the equation:

$$\frac{d^2G_l(r,r')}{dr^2}+\frac{2}{r}\frac{dG_l(r,r')}{dr}+\left(k^2-\frac{l(l+1)}{r^2}\right)G_l(r,r')=\frac{\delta(r-r')}{r^2} \tag{5}$$

The solution of this equation can be represented in terms of two independent solutions of the FSRE $j_l(kr)$ and $n_l(kr)$:

$$G_l(r,r')=\begin{cases}-kj_l(kr)\,n_l(kr') & \text{at } r<r'\\ -kj_l(kr')\,n_l(kr) & \text{at } r>r'\end{cases}, \tag{6}$$

which can be also written in equivalent form:

$$G_l(r,r') = -k\left[\theta(r'-r)\,j_l(kr)\,n_l(kr') + \theta(r-r')\,j_l(kr')\,n_l(kr)\right], \qquad (7)$$

where $\theta(x)$ is the Heaviside step function equal to 1 at positive x and 0 at negative x.The correctness of equation (5) follows from the obvious property of the $\theta-$function: $\frac{d\theta(x)}{dx} = \delta(x)$ and from the value of Wronsky determinant for spherical Bessel functions:

$$W(j_l, n_l) = \frac{dj_l}{dx}n_l - j_l\frac{dn_l}{dx} = \frac{1}{x^2} \qquad (8)$$

To ensure the correct behavior of the function $R_l(r)$ determined by equation (4) at $r \to 0$ the solution $R_l^{(0)}(r)$ of the FRSE must be chosen to be $j_l(kr)$. Thus, eq. (4) can be rewritten as follows:

$$\begin{aligned} R_l(r) &= j_l(kr) - kj_l(kr)\int\limits_r^\infty n_l(kr')\,v(r')\,R_l(r')\,r'^2dr' \\ &\quad -kn_l(kr)\int\limits_0^r j_l(kr')\,v(r')\,R_l(r')\,r'^2dr' \end{aligned} \qquad (9)$$

b) *Asymptotic behavior.*

We start with the behavior at $r \to \infty$. In this situation the first integral in eq. (9) can be neglected and the limit of integration in the second equation can be substituted by ∞. Employing the asymptotics of the spherical Bessel functions (see Mathematical Appendix 1) and the definition of the phase shift (2), we arrive at the following eqatuion expressing the phase shift in terms of integral including the exact solution $R_l(r)$:

$$\tan\delta_l = -k\int\limits_0^\infty j_l(kr)\,v(r)\,R_l(r)\,r^2dr \qquad (10)$$

At small r the lower limit in the first integral in (9) can be substituted by 0. Thus, this term as well as the first one is propostional to r^l. In the third one the factors $j_l(kr')$ and $R_l(r')$ are proportional to r'^l. If $v(r)$ is regular at $r = 0$, the integral is proportional to r^{2l+3}. Together with the factor $n_l(kr)$ it gives the result $\sim r^{l+2}$ and is small in comparison to the first two. It remains small as long as $|v(r)|$ is less singular than r^{-2}. If this condition is not satisfied, the asymptotic $R_l(r) \propto r^l$ is invalid.

c) *Scattering of slow particles.*

"Slow" means that $ka_0 \ll 1$, where $k = \sqrt{2mE}/\hbar$ is the wave vector and a_0 is the characteristic size of the potential. If the potential decreases rapidly at $r \gg a_0$ (faster than any negative power of r), then $v(r)$ restricts effectively the integration in (10) by $r \lesssim a_0$. In this range, as it follows from eq. (9), the function $R_l(r)$ has the same order of magnitude as $j_l(kr)$. Indeed, at $r \sim a_0$, the first integral in (9) can be estimated as $n_l(ka_0)\,R_l(a_0)\,v_0a_0^3$, whereas the second integral has the order of magnitude $j_l(ka_0)\,R_l(a_0)\,v_0a_0^3$. Here v_0 is the characteristic magnitude of the potential v. Thus, in this range of variables both integral terms in (9) have the same order of magnitude $\sim kj_l(ka_0)\,n_l(ka_0)\,v_0a_0^3R_l(a_0)$. At small arguments $j_l(x)\simeq\frac{2^lx^l}{(2l+1)!}$ and $n_l(x)\simeq\frac{(2l)!x^{-i-1}}{2^l}$. Thus, we find the order of magnitude of the two integral terms to be $\sim\frac{1}{2l+1}v_0a_0^2R_l(a_0)$. As a result we find that $R_l(a_0)$ differs from $j_l(ka_0)$ by a factor C which is of the order of 1 if $\frac{1}{2l+1}v_0a_0^2\lesssim 1$ or this constant is $\sim\left[\frac{1}{2l+1}v_0a_0^2\right]^{-1}$ if $\frac{1}{2l+1}v_0a_0^2\gg 1$. An important fact is that C does not depend on the wave vector k. Therefore, from eq. (10) we find $\delta_l\simeq -Ck^{2l+1}v_0a_0^{2l+3}=-C\,(ka_0)^{2l+1}\,\frac{2mV_0a_0^2}{\hbar^2}$.

So far we assumed that the potential decreases faster than any negative power of r at $r\to\infty$. Let us consider the case of the power-like decay of the potential: $v(r)\simeq v_0\left(\frac{a_0}{r}\right)^\gamma$ at $r\gg r_0$. Then all our estimates remain valid as long as $2l+3<\gamma$. We see that, at $\gamma\leq 3$, it is wrong even for the s-wave $(l=0)$. At $\gamma>3$ it is correct for $l<\frac{\gamma-3}{2}$. What happens at larger l? The integrand in equation (10) for power-like decaying potential at these values of l grows even at $r\gg a_0$ until the values $r\gtrsim l/k$ is reached. At this values of r both $j_l(kr)$ and $R_l(r)$ start to oscillate and ensure the convergence of the integral. Thus, we need to estimate the values $j_l(kr)$ and $R_l(r)$ at $r\sim k^{-1}$. Since the argument of j_l becomes of the order of 1, it is itself of the order of 1 for not very large l. In eq. (9) both integral terms at $r\sim k^{-1}$ have the order of magnitude $v_0a_0^\gamma k^{\gamma-2}R_l(1/k)$. At sufficiently small $k\ll\left(v_0a_0^\gamma\right)^{-1/(\gamma-2)}$ it can be neglected in comparison with R_l in the left-hand side of this equation. Thus, $R_l(1/k)$ also has order of magnitude 1. Then equation (10) implies that $|\delta_l|\sim k^{\gamma-2}v_0a_0^\gamma$. At large values of l the values $j_l(l)\sim R_l(l/k)\sim l^{-2/3}$ (try to prove it using semiclassical approximation). As a consequence δ_l at large l acquires an additional factor $l^{-\gamma+5/3}$ which ensures the convergence of the sum over l. At $\gamma>3$ the s-scattering remains dominant at small k. It means that $\delta_0=-ka\gg\delta_{l\neq 0}$ since, at $l\neq 0$, $\delta_l\propto k^{\beta_l}$ with $\beta_l>1$. At $2<\gamma<3$ the estimate $|\delta_0|\sim k^{\gamma-2}v_0a_0^\gamma$ is related also to $l=0$, but the series over l is divergent at least for $\theta=0$. In this case the s-scattering is not dominant and cross-section depends on angle. At $\gamma=1$ the asymptotics of spherical wave acquire a large logarithmic phase factor (we will see it when studying the Kepler -Coulomb scattering problem).

d) *Scattering phases in semiclassical approximation.*

Semiclassical approximation is correct if $ka_0\gg 1$ and $l\gg 1$. The semiclassical radial wave function reads:

$$R_l(r)=\frac{1}{r}\times\begin{cases}2k_l^{-1/2}\sin\left[\int_{r_l}^{r}k_l(r')\,dr'+\frac{\pi}{4}\right]; & r>r_l\\ |k_l|^{-1/2}\exp\left[-\int_{r}^{r_l}|k_l(r')\,dr'|\right]; & r<r_l\end{cases}, \tag{11}$$

where we introduced the local wave vector:

$$k_l(r)=\sqrt{k^2-\frac{(l+1/2)^2}{r^2}-v(r)} \tag{12}$$

and the classical turning point for radial motion r_l, which is defined as the value of r at which $k_l(r)$ turns into zero. The phase of the sinus in eq. (11) can be represented as follows:

$$\int_{r_l}^{r} k_l(r')\,dr' - \frac{\pi}{4} = \int_{r_l}^{r} \left[k_l(r') - k\right] dr' + k(r - r_l) + \frac{\pi}{4} \tag{13}$$

At $r \to \infty$, the upper limit in the integral in the r.-h. side of eq. (13) can be substituted by infinity since the integral converges if $v(r)$ decreases faster than $1/r$. Comparing this phase with that in the definition of the phase shift (2), we find the semiclassical expression for the phase shift:

$$\delta_l = \int_{r_l}^{\infty} \left[k_l(r) - k\right] dr - kr_l + \frac{(l + 1/2)\,\pi}{2} \tag{14}$$

Please, check that for a free particle $\delta_l = 0$. At very large l the turning point $r_l \approx l/k$ becomes much larger than the potential radius a_0. The difference $k_l(r) - k$ can be expanded up to linear correction in potential. It gives the asymptotic behavior of the phase shift δ_l at large $l \gg ka_0$:

$$\delta_l \approx -\frac{1}{2} \int_{r_l}^{\infty} \frac{v(r)}{k_l(r)} dr \tag{15}$$

The explicit form of this asymptotic can be obtained at additional assumptions about the asymptotic behavior of the potential $v(r)$ at large r. We consider two important cases: i) $v(r) \simeq v_0 \exp(-r/a_0)$ at $r \gg a_0$. Then $\delta_l \approx -v_0\sqrt{2\pi l a_0/k^3}\exp(-l/ka_0)$ (try to derive this formula); ii) $v(r) \simeq v_0 (a_0/r)^\gamma$ at $r \gg a_0$. In this case the resulting expression for δ_l reads:

$$\delta_l \approx -C(\gamma)\,\frac{v_0 (ka_0)^\gamma}{2l^{\gamma-1}}, \tag{16}$$

where $C(\gamma) = \sqrt{\pi}\Gamma(\gamma - 1)/\Gamma(\gamma + 1/2)$. Eq. (16) is valid at $\gamma > 1$, otherwise integral (15) diverges. The scattering amplitude $f(\theta = 0) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left(e^{2i\delta_l} - 1\right)$ and the total converges if $\gamma > 3$; the total cross section $\sigma_{tot} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l$ converges if $\gamma > 2$. Please, prove.