Phys 522 Problem Set 1
Solutions

Problem 1: Dipole matrix elements

$$\hat{H}_{int} = -\hat{\vec{d}}\cdot\vec{E}\ ,\quad \hat{\vec{d}} = -e\hat{\vec{x}}\quad \left(\text{Electric dipole operator}\right)$$

(a) Matrix elements between two energy eigenstates of the Hydrogen atom:

$$\langle n', l', m' | \hat{H}_{int} | n, l, m\rangle$$

Now recall the unitary "parity" transformation

$$\hat{\Pi}^{\dagger}\hat{\vec{x}}\,\hat{\Pi} = -\hat{\vec{x}} \Rightarrow \hat{\Pi}^{\dagger}\hat{H}_{int}\,\hat{\Pi} = -\hat{H}_{int}$$

(odd under parity)

Parity conservation ⇒ $\hat{\Pi}$ unitary

$$\hat{\Pi}^{\dagger}\hat{\Pi} = \hat{1}$$

$$\Rightarrow \langle n'l'm'|\hat{H}_{int}|nlm\rangle = \langle n'l'm'|\hat{\Pi}^{\dagger}\hat{\Pi}\,\hat{H}_{int}\,\hat{\Pi}^{\dagger}\hat{\Pi}|nlm\rangle$$

$$= -\langle n'l'm'|\hat{\Pi}^{\dagger}\hat{H}_{int}\,\hat{\Pi}|nlm\rangle$$

Aside: $\hat{\Pi}|nlm\rangle = |n,l\rangle \otimes \hat{\Pi}|l,m\rangle$

(the parity operation leaves the radial wave function unchanged since this only depends on $r^2 = |\vec{x}|^2$)

However recall that the Y_{lm}'s are eigenfunctions of parity with eigenvalue $(-1)^l$

$$\Rightarrow \hat{\Pi}|nlm\rangle = (-1)^l |n,l,m\rangle$$

$$\Rightarrow \langle n'l'm'|\hat{H}_{int}|nlm\rangle = -(-1)^{l+l'}\langle n'l'm'|\hat{H}_{int}|nlm\rangle$$

⇒ Matrix element vanishes unless

$$\boxed{(-1)^{l+l'} = -1}$$

$|n'l'm'\rangle$ and $|nlm\rangle$ must have opposite parity

(b) We write the interaction Hamiltonian in the form $\hat{H}_{int} = e\mathcal{E}_i \hat{x}_i$

where $x_1 = x$, $x_2 = y$, $x_3 = z$

The matrix element of interest is:

$$\langle \underbrace{2\,1\,m'}_{2p_m} | \hat{H}_{int} | \underbrace{1\,0\,0}_{1s_0} \rangle = e\mathcal{E}_i \langle 21m' | \hat{x}_i | 100 \rangle$$

$$= \int d^3x \; R_{21}(r) Y^*_{1m'}(\theta,\phi) \; \hat{x}_i \; R_{10}(r) Y_{00}(\theta,\phi)$$

To do these integrals, we express x, y, z in spherical coordinates, and then in spherical Harmonics.

Aside:

$x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, $z = r\cos\theta$

$$Y_{0,0}(\theta,\phi) = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{z}{r}$$

$$Y_{1,\pm1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\mp i\phi} = \mp\sqrt{\frac{3}{8\pi}}\left(x \pm iy\right)$$

$$\Rightarrow \; x = \sqrt{\frac{2\pi}{3}}\, r\left(-Y_{1,1}(\theta,\phi) + Y_{1,-1}(\theta,\phi)\right)$$

$$y = \sqrt{\frac{2\pi}{3}}\, r\left(+iY_{1,1}(\theta,\phi) + Y_{1,-1}(\theta,\phi)\right)$$

$$z = \sqrt{\frac{4\pi}{3}}\, r\, Y_{1,0}(\theta,\phi)$$

- Consider first $\vec{\mathcal{E}}$ along z

$$\langle 2p_m | \hat{H}_{int} | 1s_0 \rangle = e\mathcal{E}\sqrt{\frac{4\pi}{3}} \int_0^\infty dr\, r^3 R_{21}(r) R_{10}(r) \int d\Omega\, Y_{1,m}^* Y_{1,0} Y_{00}$$

$Y_{00} \leftarrow \sqrt{\frac{1}{4\pi}}$

$\int d\Omega\, Y_{1,m}^* Y_{1,0} = \delta_{m0}$ by orthonormality of $Y_{l,m}$'s

$$= \frac{e\mathcal{E}}{\sqrt{3}} \int dr\, r^3 R_{21}(r) R_{10}(r)\, \delta_{m,0}$$

Aside: $\int_0^\infty dr\, r^3 R_{21}(r) R_{10}(r) = a_0 \int_0^\infty d\bar{r}\, \bar{r}\, u_{21}(\bar{r}) u_{10}(\bar{r})$

where $u_{nl}(r) = r R_{nl}(r)$ (reduced radial wave function)

and $\bar{r} \equiv \frac{r}{a_0}$

For Hydrogen $u_{nl}(\bar{r}) = C_{nl}\, \bar{r}^{l+1} e^{-\frac{\bar{r}}{n}} L_{n-l-1}^{2l+1}\left(\frac{2\bar{r}}{n}\right)$

C_{nl}: Normalization

L: Laguerre polynomial

$$\Rightarrow \int_0^\infty d\bar{r}\, \bar{r}\, u_{21}(\bar{r}) u_{10}(\bar{r}) = \frac{1}{\sqrt{6}} \int_0^\infty d\bar{r}\, \bar{r}^4 e^{-\frac{3}{2}\bar{r}} \approx 1.3$$

$\Rightarrow$ For $\vec{\mathcal{E}}$ along z,

$$\langle 2p, m=0 | e\mathcal{E}\hat{z} | 1s, m=0 \rangle = (e a_0 \mathcal{E}) \frac{1.3}{\sqrt{3}} \approx 0.75\, e a_0 \mathcal{E}$$

- For $\vec{E}$ along x

$$\langle 2p, m | \hat{H}_{int} | 1s, 0 \rangle = \frac{e \mathcal{E} a_0}{\sqrt{3}} \int_0^\infty d\bar{r}\, \bar{r}\, u_{21}(\bar{r})\, u_{20}(\bar{r})$$

$$\underbrace{\int d\Omega\, Y^*_{1m} \left(\frac{-Y_{1,1}(\theta,\phi) + Y_{1,-1}(\theta,\phi)}{\sqrt{2}} \right)}$$

$$= \frac{1}{\sqrt{2}} \left(-\delta_{m,+1} + \delta_{m,-1} \right)$$

$$\Rightarrow \boxed{\begin{aligned} &\langle 2p, 0 | e\mathcal{E}\hat{x} | 1s, 0 \rangle = 0 \\ &\langle 2p, 1 | e\mathcal{E}\hat{x} | 1s, 0 \rangle = -\langle 2p, -1 | e\mathcal{E}\hat{x} | 1s, 0 \rangle \\ &\qquad = -\frac{0.75}{\sqrt{2}} e a_0 \mathcal{E} \approx 0.53\, e a_0 \mathcal{E} \end{aligned}}$$

- For $\vec{\mathcal{E}}$ along y

$$\boxed{\begin{aligned} &\langle 2p, \ \ | \qquad | 1s, 0 \rangle = 0 \\ &\langle 2p, 1 | \qquad | 1s, 0 \rangle = +\langle 2p, -1 | e\mathcal{E}\hat{y} | 1s, 0 \rangle \\ &\qquad = \frac{i}{\sqrt{2}} 0.75\, e a_0 \mathcal{E} \approx i\, 0.53\, e a_0 \mathcal{E} \end{aligned}}$$

Problem 2: Hydrogenic Atoms and Atomic Units

The system consists of two particles: a negatively charged particle 1 with charge $q_1 = -Z_1 e$ and mass m_1, and a positively charged particle 2 with charge $q_2 = Z_2 e$ and mass m_2. They interact according to the Coulomb interaction:

$$V(r) = \frac{q_1 q_2}{r} = -Z_1 Z_2 \frac{e^2}{r}$$

and their relative-motion Hamiltonian is that interaction plus a term for relative motion:

$$\hat{H}_{rel} = \frac{\hat{P}_{rel}^2}{2\mu} + V(r)$$

$$\text{where } \mu = \frac{m_1 m_2}{m_1 + m_2}$$

Combining the particles' masses and charges and the nature of their interaction, we can figure out the characteristic scales of the system:

$$\textbf{Length } l_0 = \frac{\hbar^2}{\mu q_1 q_2} = \frac{\hbar^2}{\mu Z_1 Z_2 e^2} = \left(\frac{\mathbf{m_e}}{\mu \mathbf{Z_1 Z_2}}\right)\left(\frac{\boldsymbol{\hbar^2}}{\mathbf{m_e e^2}}\right) \approx \left(\frac{me}{\mu Z_1 Z_2}\right) 0.53\mathring{A}$$

$$\textbf{Energy } E_0 = \frac{q_1 q_2}{l_0} = \left(\frac{\mu}{\mathbf{m_e}}(\mathbf{Z_1 Z_2})^{\mathbf{2}}\right)\left(\frac{\mathbf{m_e e^4}}{\boldsymbol{\hbar^2}}\right) \approx \left(\frac{\mu}{m_e}(Z_1 Z_2)^2\right) 27.2eV$$

$$\textbf{Time } t_0 = \frac{\hbar}{E_0} = \left(\frac{\mathbf{m_e}}{\mu (\mathbf{Z_1 Z_2})^{\mathbf{2}}}\right)\left(\frac{\boldsymbol{\hbar^3}}{\mathbf{m_e e^4}}\right) \approx \left(\frac{m_e}{\mu (Z_1 Z_2)^2}\right) 2.43 * 10^{-17} s$$

$$\textbf{Momentum } p_0 = \frac{\hbar}{l_0} = \left(\frac{\mu}{\mathbf{m_e}} \mathbf{Z_1 Z_2}\right)\left(\frac{\mathbf{m_e e^2}}{\boldsymbol{\hbar}}\right) \approx \left(\frac{\mu}{m_e} Z_1 Z_2\right) 2.0 * 10^{-19} g * cm/s$$

$$\textbf{Internal E-Field } \epsilon_0 = \frac{q_2}{l_0^2} = \left(\frac{\mu}{\mathbf{m_e}} \mathbf{Z_1 Z_2}\right)^{\mathbf{2}} \mathbf{Z_2} \left(\frac{\mathbf{m_e^2 e^5}}{\boldsymbol{\hbar^4}}\right) \approx \left(\left(\frac{\mu}{m_e}\right)^2 Z_1^2 Z_2^3\right) 5.7 * 10^9 V/cm$$

$$\textbf{Velocity } \frac{v_0}{c} = \frac{p_0}{\mu c} = (\mathbf{Z_1 Z_2})\left(\frac{\mathbf{e^2}}{\boldsymbol{\hbar}\mathbf{c}}\right) = (Z_1 Z_2)\alpha \approx (Z_1 Z_2)\frac{1}{137}$$

$$\textbf{Internal B-Field } B_0 = \frac{q_2}{l_0}\frac{v_0}{c} = (Z_1 Z_2)\alpha\epsilon_0 = \left(\frac{\mu}{\mathbf{m_e}}\right)^{\mathbf{2}} \mathbf{Z_1^3 Z_2^4} \left(\frac{\mathbf{m_e^2 e^7}}{\boldsymbol{\hbar^5}\mathbf{c}}\right) \approx \left(\left(\frac{\mu}{m_e}\right)^2 Z_1^3 Z_2^4\right) 10^5 G$$

$$\textbf{Magnetic Moment } M_0 = \frac{\text{current} * \text{area}}{c} = \frac{q_1}{t_0}\frac{l_0^2}{c} = \left(\frac{\mathbf{m_e}}{\mu}\mathbf{Z_1}\right)\left(\frac{\mathbf{e}\boldsymbol{\hbar}}{\mathbf{m_e c}}\right)$$

$$M_0 = \left(\frac{m_e}{\mu} Z_1\right)\mu_{Bohr} \approx \left(\frac{m_e}{\mu} Z_1\right) 1.85 * 10^{-20} erg/G$$

Note that internal E- and B-fields are calculated at particle 1, and the magnetic moment given is that of particle 1. Also note that v_0 was calculated assuming non-relativistic speeds. Now, all that remains is to plug in the values of Z_1, Z_2, and μ for each particle pair:

1. Hydrogen: $Z_1 = Z_2 = 1$, $m_1 = m_e$, $m_2 = m_p \to \mu \approx m_e$
2. Heavy (Tin) Ion: $Z_1 = 1$, $Z_2 = 50$, $m_1 = m_e$, $m_2 = m_p \to \mu \approx m_e$
3. Muonium: $Z_1 = Z_2 = 1$, $m_1 \approx 200 m_e$, $m_2 = m_p \to \mu \approx 180 m_e$
4. Positronum: $Z_1 = Z_2 = 1$, $m_1 = m_2 = m_e \to \mu = \frac{1}{2} m_e$

These values give the following numerical results:

	l_0(Å)	E_0(eV)	t_0(s)	p_0(g cm/s)	ϵ_0(V/cm)
Hydrogen	0.53	27.2	$2.4 * 10^{-17}$	$2 * 10^{-19}$	$5.7 * 10^{9}$
Heavy Ion	0.01	$6.8 * 10^{4}$	$9.6 * 10^{-21}$	10^{-17}	$7.1 * 10^{14}$
Muon + Protonμ	0.003	4896	$1.8 * 10^{-19}$	$3.6 * 10^{-17}$	$1.8 * 10^{14}$
Positronium	1.06	13.6	$4.8 * 10^{-17}$	10^{-19}	$1.4 * 10^{9}$

	v_0/c	B_0(G)	M_0(erg/G)
Hydrogen	$\frac{1}{137}$	10^{5}	$1.85 * 10^{-}20$
Heavy Ion	0.36	10^{11}	$1.85 * 10^{-}20$
Muon + Proton	$\frac{1}{137}$	$3.24 * 10^{9}$	$3.3 * 10^{-}20$
Positronium	$\frac{1}{137}$	$2.4 * 10^{4}$	$3.7 * 10^{-}20$

Problem 2: The Infinite Spherical Well and Partial Waves

We are considering solutions for spherical symmetric potentials $V(r)$. The wave function separates as

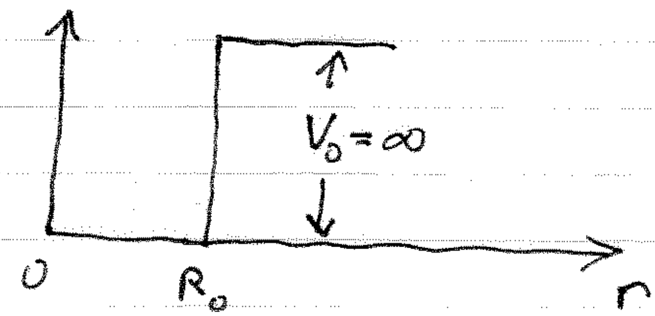
$$\psi_{n\ell m}(r,\theta,\phi) = R_{n,\ell}(r)\, Y_\ell^{m}(\theta,\phi)$$

Where the radial equation is

$$\frac{\hbar^2}{-2mr}\frac{d^2(rR)}{dr^2} + \frac{\hbar^2}{2mr^2}\ell(\ell+1)\,R(r) + V(r)\,R(r) = E\,R(r)$$

(a) Infinite potential well ("spherical box")

$$V(r) = \begin{cases} 0 & r < R_0 \\ \infty, & r > R_0 \end{cases}$$



For $r < R_0$

$$-\frac{d^2R}{dr^2} - \frac{2}{r}\frac{dR}{dr} + \frac{\ell(\ell+1)}{r^2}R = k^2 R$$

where $E \equiv (\hbar k)^2/2m$

Let $x = kr$ (dimensionless)

$$\Rightarrow \frac{d^2}{dx^2} R(x) + \frac{2}{x}\frac{dR}{dx} + \left(1 - \frac{\ell(\ell+1)}{x^2}\right) R(x) = 0$$

This is the "spherical Bessell diff'eq"
(see, e.g., Arfken, 622 – 630)

Solution $R(x) = a_\ell j_\ell(x) + b_\ell n_\ell(x)$

where $j_\ell(x) \equiv \sqrt{\frac{\pi}{2x}}\, J_{\ell+1/2}(x)$ "spherical Bessel"

$n_\ell(x) = \sqrt{\frac{\pi}{2x}}\, N_{\ell+1/2}(x)$ "spherical Neumann"

Examples:

$$j_0(x) = \frac{\sin x}{x}, \qquad n_0(x) = -\frac{\cos x}{x}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}, \qquad n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

The coefficients a_ℓ, b_ℓ are determined by the boundary conditions and normalization

Note: $j_\ell(x) \to 0$ as $x \to 0$

$|n_\ell(x)| \to \infty$ as $x \to 0$

For radial equation we have b.c. that $(rR) \to 0$ as $r \to 0$

↑ reduce wave fnct u

Thus, only the "regular solution" is allowed

$$R(x) = a_\ell j_\ell(x) \Rightarrow R(r) = a_\ell \sqrt{k}\, j_\ell(kr)$$
(with dimensions)

Finally, we have the b.c. at $r = R_0$ or $x = kR_0$

$\Rightarrow$ The energy eigenvalues are the (discrete set) roots of the spherical Bessel fnct.

$$\boxed{E_{n,\ell} = \frac{(\hbar k_{n,\ell})^2}{2m}, \text{ where } j_\ell(k_{n,\ell} R_0) = 0}$$

$\uparrow$ $2\ell+1$ degenerate

$$\Rightarrow \boxed{\psi_{n,\ell,m}(r,\theta,\phi) = A_{n\ell,m}\, j_\ell(k_{n,\ell} r)\, Y_\ell^m(\theta,\phi)}$$

Normalization: $\int d^3x\, |\psi_{n,\ell,m}(\vec{x})|^2 = 1$

$$\Rightarrow A_{n,\ell,m}^2 \underbrace{\int_0^{R_0} r^2 dr \left[j_\ell(k_{n,\ell} r)\right]^2}_{} = 1$$

$\frac{R_0^3}{2}\left[j_{\ell+1}(k_{n\ell}R_0)\right]^2$ (from Arfken 11.169)

$\qquad \| $

$\qquad -j_\ell'(k_{n,\ell}R_0)$ (from Arfken 11.162)

$$\Rightarrow \boxed{A_{n,\ell,m} = \left(\frac{2}{R_0^3}\,\frac{1}{j_\ell'(k_{n\ell}R_0)}\right)^{1/2}}$$

(b) In the limit $R_0 \to \infty$ we have a free particle. The spectrum become continuous

$$E(k) = \frac{(\hbar k)^2}{2m} \quad , \quad \psi_{k,l,m}(r,\theta,\phi) = A(k)\, j_l(kr)\, Y_l^m(\theta,\phi)$$

$\uparrow$ continuous parameter

This should be contrasted with the plane wave

$$\psi_{\vec{k}}(\vec{x}) = A_{\vec{k}}\, e^{i\vec{k}\cdot\vec{x}} \qquad E(\vec{k}) = \frac{(\hbar|\vec{k}|)^2}{2m}$$

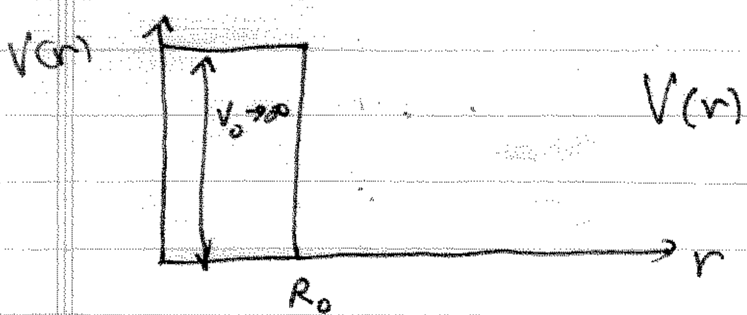
These are two different choices because of the degeneracy; the energy eigenvalue depends on $|\vec{k}|$, not its direction.

- The plane waves are simultaneous eigenvectors of $\hat{P}_x, \hat{P}_y, \hat{P}_z$, all of which commute with $\hat{H}_{free}$

- The "partial waves" are simultaneous eigenvectors of $\hat{H}_{free}, \hat{L}^2, \hat{L}_z$

Note $[\hat{P}_i, \hat{L}_z] \neq 0$ so these are two different bases. they both represent two complete sets, so a plane wave can be expanded in partial waves etc.

(c) Now we consider the "hard sphere"



$$V(r) = \begin{cases} \infty & r < R_0 \\ 0 & r > 0 \end{cases}$$

Outside the sphere, the particle is free. But, since the origin is not included, we must use <u>both</u> the regular and irregular solution to be general and match the b.c.

$$\psi_{k,l,m}(r,\theta,\phi) = \underbrace{\left(A_l(k) j_l(kr) + B_l(k) n_l(kr)\right)}_{R_{k,l}(r)} Y_l^m(\theta,\phi)$$

b.c. $R_{k,l}(R_0) = 0 \Rightarrow \boxed{\dfrac{B_l(k)}{A_l(k)} = -\dfrac{j_l(kR_0)}{n_l(kR_0)}}$

(d) For s-waves, i.e. $l=0$

$$R_{kl}(r) = A_0(k)\left(j_0(kr) + \frac{B_0(k)}{A_0(k)} n_0(kr) \right)$$

$$= \frac{A_0(k)}{n_0(kR_0)} \left(j_0(kr)\, n_0(kR_0) - n_0(kr)\, j_0(kR_0) \right)$$

$$= \frac{A_0(k)}{(kR_0)\, n_0(kR_0)} \left(\frac{-\sin(kr)\cos(kR_0) + \cos(kr)\sin(kR_0)}{kr} \right)$$

(Next Page)

$$\Rightarrow R_{k,\ell}(r) = C(k) \frac{\sin(k(r-R_0))}{kr}$$

where $$C(k) = \frac{-A(k)}{kR_0\, n_0(kR_0)}$$

the "reduced" radial wave function

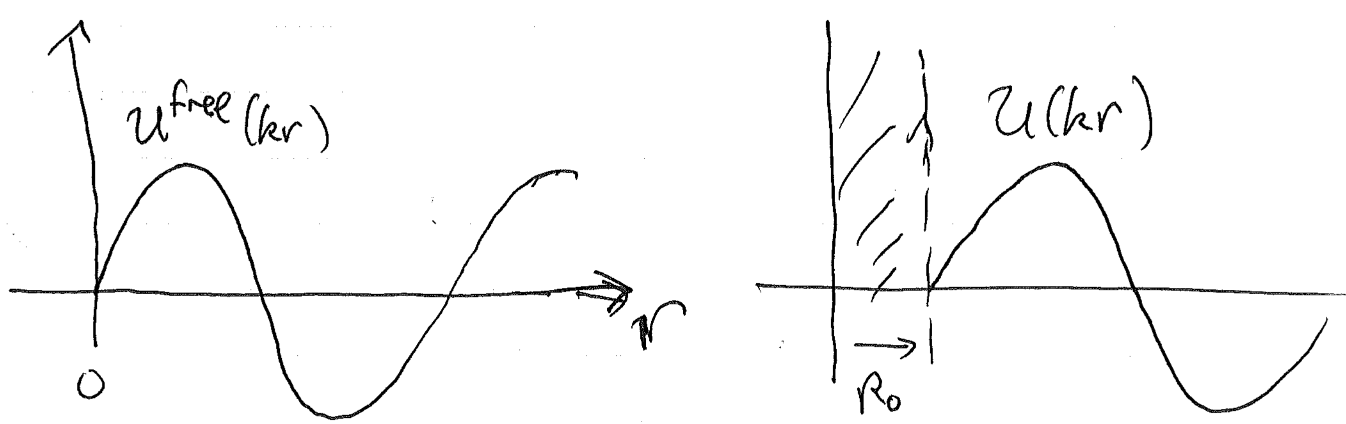
$$u_{k,\ell}(kr) = r\, R_{k\ell}(r) = C(k) \sin(kr - kR_0)$$

For a free particle with $\ell = 0$

$$u^{free}_{k,0}(kr) = C(k) \sin(kr)$$

$$\Rightarrow \boxed{u_{k,\ell}(kr) = u^{free}_{k,\ell}(kr + \delta_0) \qquad \delta_0 = -kR_0}$$

Graphically



The effect of the hard-sphere is a phase-shift