

8.322: Quantum Theory II

Problem Set #11 Solutions

May 14, 2007

1. A formula for the phase shift

(a) We have

$$f(\vec{k}, \vec{k}') = \sum_l (2l+1) f_l(k) P_l(\cos \theta_{\vec{k}, \vec{k}'}) = -\frac{2m}{4\pi} \langle \vec{k}' | V | \psi_{\vec{k}}^{(+)} \rangle$$

Now

$$\begin{aligned} \langle \vec{k}' | V | \psi_{\vec{k}}^{(+)} \rangle &= \int \int \langle \vec{k}' | \vec{x} \rangle \langle \vec{x} | V | \vec{x}' \rangle \langle \vec{x}' | \psi_{\vec{k}}^{(+)} \rangle d^3 \vec{x}' d^3 \vec{x} \\ &= \int \langle \vec{x} | \vec{k}' \rangle^* V(\vec{x}) \langle \vec{x} | \psi_{\vec{k}}^{(+)} \rangle d^3 \vec{x} \\ &= \int e^{-i\vec{k}' \cdot \vec{x}} V(\vec{x}) \sum_l (2l+1) i^l e^{i\delta_l(k)} P_l(\cos \theta_{\vec{k}, \vec{x}}) R_l(k, r) d^3 \vec{x} \\ &= \sum_l (2l+1) i^l e^{i\delta_l(k)} \int_0^\infty r^2 dr \int d\Omega e^{-i\vec{k}' \cdot r \cos \theta_{\vec{k}', \vec{x}}} V(r) P_l(\cos \theta_{\vec{k}, \vec{x}}) R_l(k, r) \end{aligned}$$

where we used the following:

$$\langle \vec{x} | \psi_{\vec{k}}^{(+)} \rangle = \sum_l (2l+1) i^l e^{i\delta_l(k)} P_l(\cos \theta_{\vec{k}, \vec{x}}) R_l(k, r)$$

Since the scattering is elastic, $|\vec{k}| = |\vec{k}'|$. We also know that

$$e^{-i\vec{k}' \cdot r \cos \theta_{\vec{k}', \vec{x}}} = \sum_{l'} (2l'+1) (-i)^{l'} P_{l'}(\cos \theta_{\vec{k}', \vec{x}}) j_{l'}(k'r)$$

Substituting this and using the following addition formula

$$\int d\Omega P_l(\cos \theta_{\vec{k}, \vec{x}}) P_{l'}(\cos \theta_{\vec{k}', \vec{x}}) = \frac{4\pi \delta_{l,l'}}{2l+1} P_l(\cos \theta_{\vec{k}, \vec{k}'})$$

gives

$$\langle \vec{k}' | V | \psi_{\vec{k}}^{(+)} \rangle = 4\pi \sum_l (2l+1) e^{i\delta_l(k)} P_l(\cos \theta_{\vec{k}, \vec{k}'}) \left(\int_0^\infty r^2 V(r) j_l(kr) R_l(k, r) dr \right)$$

Now since

$$f_l(k) = \frac{e^{i\delta_l(k)}}{k} \sin \delta_l(k)$$

we obtain our final expression

$$\sin \delta_l(k) = -2mk \int_0^\infty r^2 V(r) j_l(kr) R_l(k, r) dr$$

(b) In the absence of the potential,

$$R_l(k, r) = j_l(kr)$$

therefore to first order we have

$$\sin \delta_l(k) = -2mk \int_0^\infty r^2 dr j_l^2(kr) V(r)$$

(c) Since $\sin \delta_l^{1BA}$ is linear in V , we can always rescale the potential s. t.

$$\sin \delta_l^{1BA} > 1$$

However, this should not surprise us since we used only the first Born approximation of the true δ_l . When the bound is not satisfied, the approximation fails anyway. To obtain the correct bound, we need to take into account all the higher order corrections in general.

2. Scattering from an atom in the first Born approximation

(a)

$$q = |\vec{k} - \vec{k}'| = \sqrt{|\vec{k}|^2 + |\vec{k}'|^2 - 2|\vec{k}||\vec{k}'| \cos \theta}$$

Since $|\vec{k}| = |\vec{k}'|$,

$$q = |\vec{k}| \sqrt{2(1 - \cos \theta)}$$

$$q = 2|\vec{k}| \sin \frac{\theta}{2}$$

(b) In the first Born approximation, the scattering amplitude is

$$f(\vec{k}, \vec{k}') = -\frac{2m}{4\pi} \langle \vec{k}' | V | \vec{k} \rangle = -\frac{2m}{4\pi} \int e^{-i\vec{k}' \cdot \vec{x}} V(\vec{x}) e^{i\vec{k} \cdot \vec{x}} d^3 \vec{x} = -\frac{2m}{4\pi} \int V(\vec{x}) e^{i\vec{q} \cdot \vec{x}} d^3 \vec{x}$$

The potential due to the charge distribution is given by

$$V(\vec{x}) = -\frac{Ze^2}{|\vec{x}|} + \int \frac{e^2 \rho(\vec{x}')}{|\vec{x} - \vec{x}'|} d^3 \vec{x}'$$

where the first term comes from the nucleus and the second term from the electron density.

Hence,

$$f(\vec{k}, \vec{k}') = -\frac{2me^2}{4\pi} \left[-Z \int \frac{e^{i\vec{q} \cdot \vec{x}}}{|\vec{x}|} d^3 \vec{x} + \int \int \frac{\rho(\vec{x}') e^{i\vec{q} \cdot \vec{x}}}{|\vec{x} - \vec{x}'|} d^3 \vec{x} d^3 \vec{x}' \right]$$

Now

$$\int \frac{e^{i\vec{q}\cdot\vec{x}}}{|\vec{x}|} d^3\vec{x} = \frac{4\pi}{q^2}$$

and

$$\int \int \frac{\rho(\vec{x}') e^{i\vec{q}\cdot\vec{x}}}{|\vec{x} - \vec{x}'|} d^3\vec{x} d^3\vec{x}' = \int d^3\vec{x}' \rho(\vec{x}') \int d^3\vec{x} \frac{e^{i\vec{q}\cdot\vec{x}}}{|\vec{x} - \vec{x}'|} = \frac{4\pi}{q^2} \int e^{i\vec{q}\cdot\vec{x}'} \rho(\vec{x}') d^3\vec{x}'$$

Combining,

$$\begin{aligned} f(\vec{k}, \vec{k}') &= -\frac{2me^2}{4\pi} \left[-\frac{4\pi Z}{q^2} + \frac{4\pi}{q^2} \int e^{i\vec{q}\cdot\vec{x}} \rho(\vec{x}) d^3\vec{x} \right] \\ &= \frac{2}{q^2} \underbrace{(me^2)}_{1/a_0} (Z - F(\vec{q})) \end{aligned}$$

where

$$F(\vec{q}) = \int e^{i\vec{q}\cdot\vec{x}} \rho(\vec{x}) d^3\vec{x}$$

is the form factor and a_0 is the Bohr radius. Then,

$$\frac{d\sigma}{d\Omega} = |f(\vec{k}, \vec{k}')|^2 = \left(\frac{2}{a_0 q^2} \right)^2 (Z - F(\vec{q}))^2$$

(c) Assuming that the charge density is spherically symmetric,

$$\begin{aligned} F(\vec{q}) &= \int e^{iqr \cos \theta} \rho(r) r^2 \sin \theta dr d\theta d\phi \\ \frac{d^2 F(q)}{dq^2} &= \int (ir \cos \theta)^2 e^{iqr \cos \theta} \rho(r) r^2 \sin \theta dr d\theta d\phi \\ \left. \frac{d^2 F}{dq^2} \right|_{q=0} &= \int (ir \cos \theta)^2 \rho(r) r^2 \sin \theta dr d\theta d\phi = -\frac{4\pi}{3} \int_0^\infty r^4 \rho(r) dr \end{aligned}$$

On the other hand,

$$\langle r^2 \rangle = \int r^2 \rho(r) d^3\vec{x} = 4\pi \int_0^\infty r^2 \rho(r) r^2 dr$$

Comparing,

$$\left. \frac{d^2 F(q)}{dq^2} \right|_{q=0} = -\frac{1}{3} \langle r^2 \rangle$$

F can be regarded as a function of q^2 . By symmetry, odd derivatives of F with respect to q vanish and we have

$$\left. \frac{dF(q^2)}{d(q^2)} \right|_{q=0} = \frac{1}{2!} \left. \frac{d^2 F(q)}{dq^2} \right|_{q=0} = -\frac{1}{6} \langle r^2 \rangle$$

In the forward scattering limit $\vec{k} \approx \vec{k}'$. Hence, $\vec{q} \approx 0$.

$$\begin{aligned} \left. \frac{d\sigma}{d\Omega} \right|_{\theta \rightarrow 0} &= \lim_{q \rightarrow 0} \left(\frac{2}{a_0 q^2} \right)^2 (Z - F(\vec{q}))^2 \\ &= \lim_{q \rightarrow 0} \left\{ \left(\frac{2}{a_0 q^2} \right)^2 \left(Z - \underbrace{[F(0)]}_Z - \frac{1}{6} \langle r^2 \rangle q^2 + \mathcal{O}(q^4) \right)^2 \right\} \\ &= \lim_{q \rightarrow 0} \left(\frac{\langle r^2 \rangle}{3a_0} + \mathcal{O}(q^2) \right)^2 = \left(\frac{\langle r^2 \rangle}{3a_0} \right)^2 \end{aligned}$$

(d) For hydrogen,

$$\rho(r) = \frac{1}{\pi a_0^3} e^{-2r/a_0}$$

The form factor is

$$\begin{aligned} F(q) &= \int \frac{1}{\pi a_0^3} e^{-2r/a_0} e^{iqr \cos \theta} r^2 dr d(\cos \theta) d\phi \\ &= \frac{2}{a_0^3} \int_0^\infty \left(\frac{e^{iqr} - e^{-iqr}}{iqr} \right) e^{-2r/a_0} r^2 dr = \frac{2}{iqa_0^3} \left[\frac{1}{(\frac{2}{a_0} - iq)^2} - \frac{1}{(\frac{2}{a_0} + iq)^2} \right] = \frac{16}{(4 + a_0^2 q^2)^2} \end{aligned}$$

Next,

$$\langle r^2 \rangle = 4\pi \int_0^\infty r^4 \rho(r) dr = \frac{4}{a_0^3} \int_0^\infty r^4 e^{-2r/a_0} dr = 3a_0^2$$

We can check the relation in (c)

$$\left. \frac{dF}{dq^2} \right|_{q=0} = - \frac{32a_0^2}{(4 + a_0^2 q^2)^3} \Big|_{q=0} = - \frac{a_0^2}{2} = - \frac{1}{6} (3a_0^2)$$

(e) We first calculate ρ_0 as a function of Z and A and find

$$\rho_0 = \frac{3Z}{4\pi R_0^3 A}$$

We now calculate the form factor $F(\vec{q})$ for this charge distribution

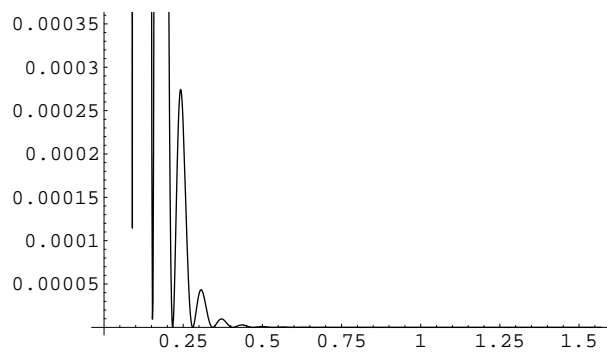
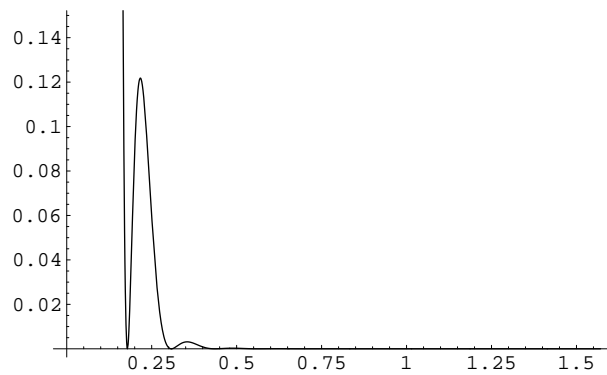
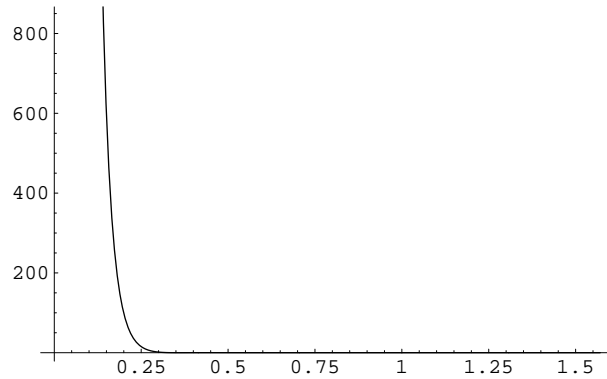
$$\begin{aligned} F(\vec{q}) &= \int d^3x e^{i\vec{q}\cdot\vec{x}} \rho(\vec{x}) \\ &= \frac{4\pi\rho_0}{q} \int_0^{R_0 A^{1/3}} r \sin(qr) dr \\ &= \frac{4\pi\rho_0}{q^3} [-qR_0 A^{1/3} \cos(qR_0 A^{1/3}) + \sin(qR_0 A^{1/3})] \\ &= \frac{3Z}{q^3 R_0^3 A} [-qR_0 A^{1/3} \cos(qR_0 A^{1/3}) + \sin(qR_0 A^{1/3})] \end{aligned}$$

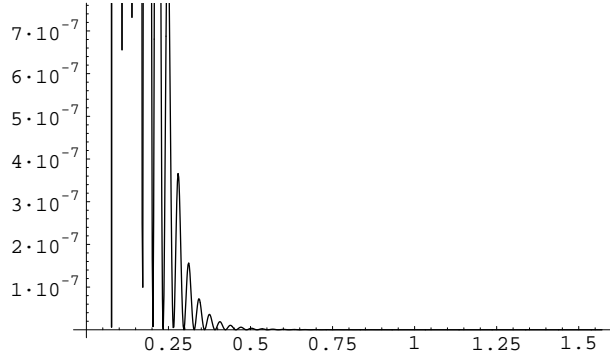
We then use the earlier result that the differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \left(\frac{2}{a_0 q^2} \right)^2 F(\vec{q})^2$$

and plug in that $q = 2k \sin(\theta/2)$.

(f) Plotted in order of increasing energy (\vec{k}).





(g) Smearing out the surface of the nucleus, leads to a change in the large q behavior of the cross-section. In particular, the cross-section will decrease faster for a smooth boundary and will decay exponentially rather than as a power-law.

3. Born Approximation for a δ -shell

(a) We have

$$f(k, \theta) = -\frac{2m}{4\pi} \int e^{i\vec{q}\cdot\vec{x}} V(\vec{x}) d^3\vec{x}$$

where $\vec{q} = \vec{k} - \vec{k}'$ such that $q = 2k \sin(\theta/2)$.

Substituting the potential $2mV(r) = -\lambda\delta(r - a)$,

$$f(k, \theta) = \frac{\lambda}{4\pi} \int e^{i\vec{q}\cdot\vec{x}} \delta(r - a) d^3\vec{x} = \frac{\lambda}{4\pi} \int r^2 dr 4\pi \frac{\sin(qr)}{qr} \delta(r - a)$$

$$f(k, \theta) = \frac{\lambda a}{q} \sin(qa) = \frac{\lambda a}{2k \sin(\theta/2)} \sin \left[2ka \sin \frac{\theta}{2} \right]$$

(b) See Fig. 1

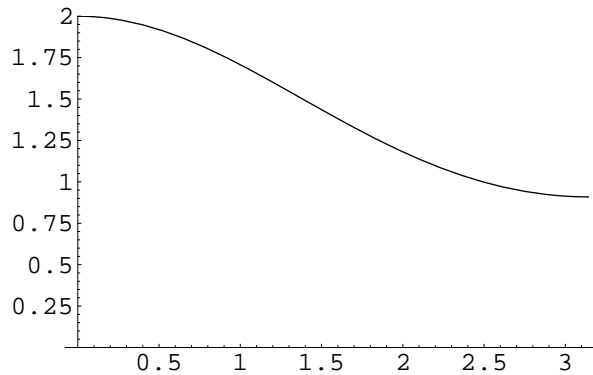


Figure 1: The scattering amplitude $f(k, \theta)$ as a function of $\theta \in [0, \pi]$. ($\lambda = 2$, $a = k = 1$.)

(c) Recall

$$f(k, \theta) = \sum_l (2l + 1) f_l(k) P_l(\cos \theta)$$

Using the orthonormality of P_l ,

$$2f_0(k) = \int_{-1}^1 d(\cos \theta) P_0(\cos \theta) \left[\sum_l (2l + 1) f_l(k) P_l(\cos \theta) \right] = \int_{-1}^1 d(\cos \theta) P_0(\cos \theta) f(k, \theta)$$

Hence,

$$\begin{aligned} f_0(k) &= \frac{1}{2} \int_0^\pi \frac{\lambda a}{2k \sin(\theta/2)} \sin \left[2ka \sin \frac{\theta}{2} \right] \sin \theta \, d\theta \\ &= 2 \int_0^\pi \frac{\lambda a}{2k} \sin(2ka \sin \theta/2) d \left(\sin \frac{\theta}{2} \right) = \frac{\lambda}{2k^2} (1 - 2 \cos(2ka)) \\ f_0(k) &= \frac{\lambda}{k^2} \sin^2(ka) \end{aligned} \tag{0.1}$$

Now

$$e^{2i\delta_l(k)} = 1 + 2ik f_l(k)$$

Combining with (0.1) this gives

$$\tan 2\delta_0(k) = \frac{2\lambda}{k} \sin^2(ka) \tag{0.2}$$

For small k

$$\delta_0(k) \approx \lambda a^2 k$$

(d) The solution to the Schrödinger equation

$$\psi(\vec{x}) = Y_{lm}(\theta, \phi) R_l(r)$$

where $R_l(r) \equiv r \cdot u(r)$. For the s-wave,

$$\left(-\frac{1}{2m} \frac{d^2}{dr^2} + V(r) \right) u(r) = E u(r)$$

Substituting the potential

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

gives

$$u'' + \lambda \delta(r - a) u + k^2 u = 0$$

with $k = \sqrt{2mE}$. For $r \neq a$, we have the solution

$$u(r) = A \sin(kr) + B \cos(kr)$$

For $r < a$ we demand the radial wavefunction $u(r)$ to vanish at $r = 0$

$$u(r) \sim \sin(kr)$$

For $r > a$ we have a phase shift

$$u(r) \sim \sin(kr + \delta_0(k))$$

At $r = a$, $u(r)$ must be continuous. Moreover, integrating from $a - 0$ to $a + 0$ gives

$$u'(a + 0) - u'(a - 0) + \lambda u(a) = 0$$

This yields

$$\cot(ka) - \cot(ka + \delta_0(k)) = \frac{\lambda}{k}$$

Finally,

$$\delta_0(k) = \operatorname{arccot} \left(\cot(ka) - \frac{\lambda}{k} \right) - ka \quad (0.3)$$

We can see the deviance of the Born approximated phase shift from the exact value by plotting the two functions (0.2) and (0.3). See Figure 2 and Figure 3.

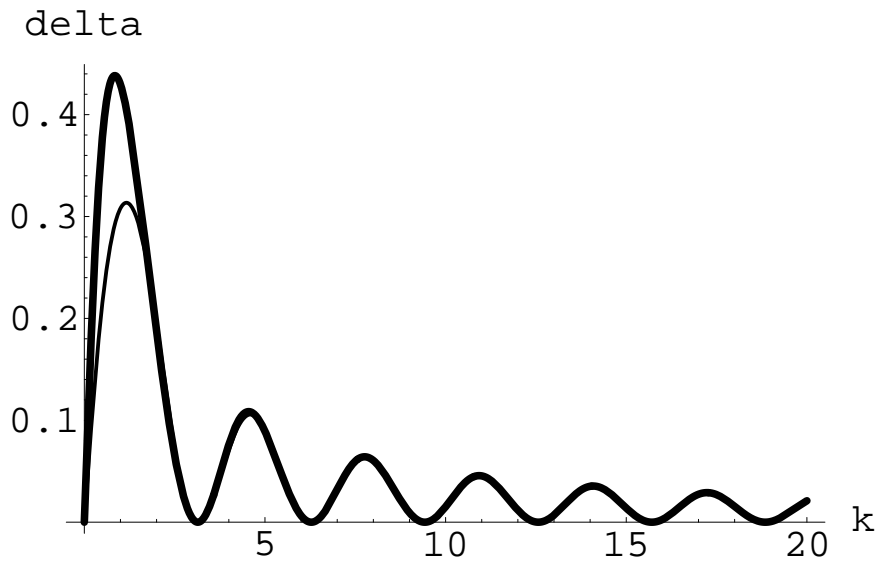


Figure 2: The exact (thick line) and the Born approximated (thin line) phase shifts for $a = 1$ and $\lambda = 1/2$.

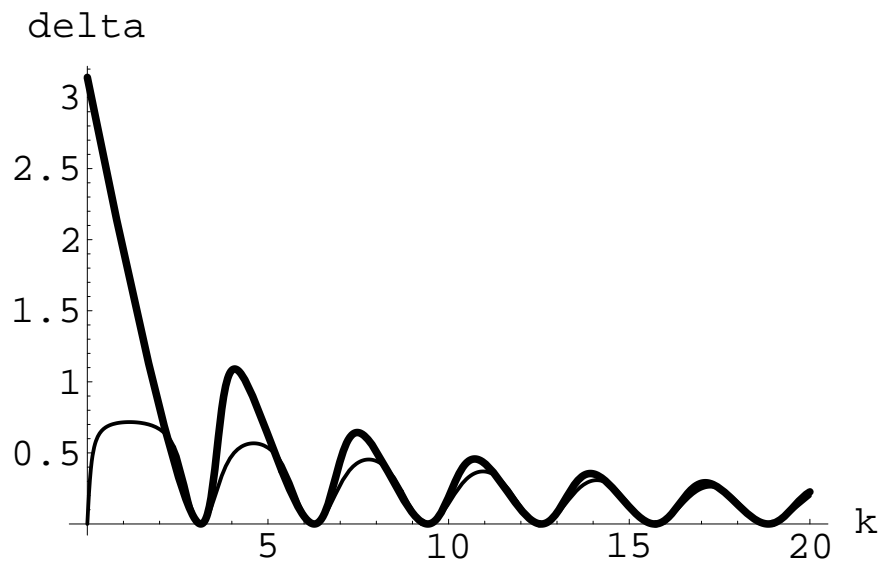


Figure 3: The phase shifts for $a = 1$ and $\lambda = 5$. The system has a bound state since $\delta_0(k) \rightarrow \pi$ as $k \rightarrow 0$. The Born approximation fails to capture this.

4. Spin dependent scattering

(a) For the two-component spinor wavefunction $\begin{pmatrix} \psi^\uparrow \\ \psi^\downarrow \end{pmatrix}$ the time-independent Schrödinger equation is

$$-\frac{1}{2m}\nabla^2\begin{pmatrix} \psi^\uparrow \\ \psi^\downarrow \end{pmatrix} + \underbrace{\begin{pmatrix} V(\vec{x}) & W(\vec{x}) \\ W(\vec{x}) & 0 \end{pmatrix}}_{V_0}\begin{pmatrix} \psi^\uparrow \\ \psi^\downarrow \end{pmatrix} = E\begin{pmatrix} \psi^\uparrow \\ \psi^\downarrow \end{pmatrix}$$

(b) The Lippmann-Schwinger equation,

$$|\psi_{\vec{k},s}^{(+)}\rangle = |\phi_{\vec{k},s}\rangle + \frac{1}{E - H_0 + i\epsilon}V_0|\psi_{\vec{k},s}^{(+)}\rangle$$

gives

$$\psi_{\vec{k},s}^{(+)}(\vec{x}) = \phi_{\vec{k},s}(\vec{x}) + \int \underbrace{\langle\vec{x}|\frac{1}{E - H_0 + i\epsilon}|\vec{x}'\rangle}_{G_0^{(+)}(\vec{x},\vec{x}',E)}\langle\vec{x}'|V_0|\psi_{\vec{k},s}^{(+)}\rangle d^3\vec{x}'$$

where

$$G_0^{(+)}(\vec{x},\vec{x}',E) = -\frac{2m}{4\pi}\frac{e^{ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}$$

(c) By definition,

$$f_{\uparrow\uparrow}(\vec{k},\vec{k}') = -\frac{2m}{4\pi}\langle\phi_{\vec{k}',\uparrow}|V_0|\psi_{\vec{k},\uparrow}^{(+)}\rangle = -\frac{2m}{4\pi}\left[\langle\vec{k}'|V|\psi_{\vec{k},\uparrow}^\uparrow\rangle + \langle\vec{k}'|W|\psi_{\vec{k},\uparrow}^\downarrow\rangle\right]$$

(Here $\psi_{\vec{k},\uparrow}^{\uparrow/\downarrow}$ are the two components of the spinor $\psi_{\vec{k},\uparrow}^{(+)}$.)

The first Born approximation takes $|\psi_{\vec{k},\uparrow}^{(+)}\rangle = |\phi_{\vec{k},\uparrow}\rangle$. Then,

$$f_{\uparrow\uparrow}(\vec{k},\vec{k}') = -\frac{2m}{4\pi}\left[\langle\vec{k}'|V|\vec{k}\rangle + 0\right] = -\frac{2m}{4\pi}\int d^3\vec{x}e^{-i\vec{k}'\cdot\vec{x}}V(\vec{x})e^{i\vec{k}\cdot\vec{x}} = -\frac{2m}{4\pi}\tilde{V}(\vec{k}' - \vec{k})$$

Next,

$$f_{\uparrow\downarrow}(\vec{k},\vec{k}') = -\frac{2m}{4\pi}\langle\phi_{\vec{k}',\downarrow}|V|\psi_{\vec{k},\uparrow}^{(+)}\rangle = -\frac{2m}{4\pi}\langle\vec{k}'|W|\psi_{\vec{k},\uparrow}^\uparrow\rangle = -\frac{2m}{4\pi}\tilde{W}(\vec{k}' - \vec{k})$$

Similarly,

$$f_{\downarrow\uparrow}(\vec{k},\vec{k}') = -\frac{2m}{4\pi}\tilde{W}(\vec{k}' - \vec{k})$$

Finally,

$$f_{\downarrow\downarrow}(\vec{k},\vec{k}') = -\frac{2m}{4\pi}\langle\phi_{\vec{k}',\downarrow}|V|\psi_{\vec{k},\downarrow}^{(+)}\rangle$$

To first order this is zero since $|\psi_{\vec{k},\downarrow}^\uparrow\rangle = 0$. Hence, we need to consider the 2nd order correction,

$$|\psi_{\vec{k},\downarrow}^\uparrow\rangle = \frac{1}{E - H_0 + i\epsilon}\left(V\cdot 0 + W|\vec{k}'\rangle\right)$$

Hence,

$$f_{\downarrow\downarrow}(\vec{k}, \vec{k}') = -\frac{2m}{4\pi} \langle \vec{k}' | W \frac{1}{E - H_0 + i\epsilon} W | \vec{k} \rangle = -\frac{2m}{4\pi} \int \frac{d^3\vec{p}}{(2\pi)^3} \tilde{W}(\vec{p} - \vec{k}') \frac{1}{k^2/2m - p^2/2m + i\epsilon} \tilde{W}(\vec{k} - \vec{p})$$