APPENDIX

For the 2 lectures of Claude Cohen-Tannoudji
on “Atom-Atom Interactions
in Ultracold Quantum Gases”

Purpose of this Appendix

1 – Demonstrate the orthonormalization relation

$$\langle \varphi_{k'l'm'} | \varphi_{klm} \rangle = \delta(k - k')\delta_{ll'}\delta_{mm'} \qquad \textbf{(A.1)}$$

- The wave function

$$\varphi_{klm}(\vec{r}) = \sqrt{\frac{2}{\pi}}\frac{u_{kl}(r)}{r} Y_{lm}(\theta,\varphi) \qquad \textbf{(A.2)}$$

describes, in the angular momentum representation, a particle of mass μ, with energy $E=\hbar^2 k^2/2\mu$, in a central potential $V(r)$

- The radial wave function $u_{kl}(r)$ is a regular solution of

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{2\mu}{\hbar^2}V_{\text{tot}}(r)\right] u_{k\,l}(r) = 0 \qquad V_{\text{tot}}(r) = V(r) + \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2} \qquad \textbf{(A.3)}$$

$$u_{kl}(0) = 0 \qquad \textbf{(A.4)}$$

which behaves, for r→∞, as:

$$u_{kl}(r) \underset{r\to\infty}{\simeq} \sin\left[kr - l\pi/2 + \delta_l(k)\right] \qquad \textbf{(A.5)}$$

- There are other (non regular) solutions behaving, for r→∞, as:

$$u_{kl}^{\pm}(r) \underset{r\to\infty}{\simeq} \exp\left[\pm i\left(k\,r - l\pi/2\right)\right] = (\mp i)^l \exp(\pm ikr) \qquad \textbf{(A.6)}$$

2 – Calculate the Green function of: $H = p^2/2\mu + V(r)$

with outgoing and ingoing asymptotic behavior

$$\left(E - H\right) G^{(\pm)}\left(\vec{r}, \vec{r}'\right) = \delta\left(\vec{r} - \vec{r}'\right) \qquad E = \hbar^2 k^2 / 2\mu \tag{A.7}$$

- Show that:

$$G^{(\pm)}\left(\vec{r}, \vec{r}'\right) = -\frac{2\mu}{\hbar^2}\frac{1}{krr'}\sum_{lm}\exp(\pm i\,\delta_l)\,Y^*_{lm}(\theta,\varphi)Y_{lm}(\theta',\varphi')u_{kl}(r_<)u^{\pm}_{kl}(r_>) \tag{A.8}$$

where $r_>$ ($r_<$) is the largest (smallest) of r and r'

- Introducing the Heaviside function:

$$\theta\left(r - r'\right) = +1 \quad \text{if} \quad r > r'$$
$$= 0 \quad \text{if} \quad r < r' \tag{A.9}$$

(A.8) can also be written:

$$G^{(\pm)}\left(\vec{r}, \vec{r}'\right) = -\frac{2\mu}{\hbar^2}\frac{1}{krr'}\sum_{lm}\exp(\pm i\,\delta_l)\,Y^*_{lm}(\theta,\varphi)Y_{lm}(\theta',\varphi') \times$$
$$\times\left[\theta\left(r - r'\right)u_{kl}(r')u^{\pm}_{kl}(r) + \theta\left(r' - r\right)u_{kl}(r)u^{\pm}_{kl}(r')\right] \tag{A.10}$$

3 – Calculate the asymptotic behavior of these Green functions

and demonstrate Equation (2.39) of Lecture 2

Wronskian Theorem

The calculations presented in this Appendix use the Wronskian theorem (see demonstration in Ref.2 Chapter III-8)

- Consider the 1D second order differential equation:

$$y''(r) + F(r)y(r) = 0 \tag{A.11}$$

Equation (A.4) is of this type with:

$$F(r) = k^2 - \frac{2\mu}{\hbar^2} V_{\text{tot}}(r) \tag{A.12}$$

- Let $y_1(r)$ and $y_2(r)$ be 2 solutions of this equation corresponding to 2 different functions $F_1(r)$ and $F_2(r)$, respectively.

The wronskian of y_1 and y_2 is by definition:

$$W(y_1, y_2) = y_1(r)y_2'(r) - y_2(r)y_1'(r) \tag{A.13}$$

- One can show that:

$$W(y_1, y_2)\Big|_a^b = \left[W(y_1, y_2)\right]_{r=b} - \left[W(y_1, y_2)\right]_{r=a} = \int_a^b \left[F_1(r) - F_2(r)\right] y_1(r)\, y_2(r)\, \mathrm{d}r \tag{A.14}$$

Demonstration of (A.1)

We consider 2 different values k_1 and k_2 of k. According to (A.12):

$$\boldsymbol{F}_1(\boldsymbol{r}) - \boldsymbol{F}_2(\boldsymbol{r}) = \boldsymbol{k}_1^2 - \boldsymbol{k}_2^2 \qquad \textbf{(A.15)}$$

(A.14) then gives the scalar product of $y_1 = u_{k_1 l}$ and $y_2 = u_{k_2 l}$

$$\int_a^b \boldsymbol{y}_1(\boldsymbol{r})\, \boldsymbol{y}_2(\boldsymbol{r})\, \mathrm{d}\boldsymbol{r} = \frac{1}{\boldsymbol{k}_1^2 - \boldsymbol{k}_2^2} \boldsymbol{W}(\boldsymbol{y}_1, \boldsymbol{y}_2)\Big|_a^b \qquad \textbf{(A.16)}$$

If we take $a = 0$, $\left[W(y_1, y_2)\right]_{r=a} = 0$ because of (A.4)

If we take $b = R$ very large compared to the range of $V(r)$, we can use the asymptotic behavior (A.5) of $u_{k_1 l}$ and $u_{k_2 l}$

$$\int_0^R u_{k_1 l}(r)\, u_{k_2 l}(r)\, \mathrm{d}r = \frac{1}{k_1^2 - k_2^2}\left[u_{k_1 l}(r) u'_{k_2 l}(r) - u_{k_2 l}(r) u'_{k_1 l}(r)\right]_{r=R} \qquad \textbf{(A.17)}$$

Using (A.15) and putting $\delta_l(k_1) = \delta_1$, $\delta_l(k_2) = \delta_2$, we get:

$$\int_0^R \boldsymbol{u}_{k_1 l}(\boldsymbol{r})\, \boldsymbol{u}_{k_2 l}(\boldsymbol{r})\, \mathrm{d}\boldsymbol{r} = -\frac{1}{2}\frac{\sin\left[\left(\boldsymbol{k}_1 + \boldsymbol{k}_2\right)\boldsymbol{R} - \ell\pi + \delta_1 + \delta_2\right]}{\boldsymbol{k}_1 + \boldsymbol{k}_2} + \frac{1}{2}\frac{\sin\left[\left(\boldsymbol{k}_1 - \boldsymbol{k}_2\right)\boldsymbol{R} + \delta_1 - \delta_2\right]}{\boldsymbol{k}_1 - \boldsymbol{k}_2} \qquad \textbf{(A.18)}$$

- When R→∞, the first term of the right side of (A.18) vanishes as a distribution, because it is a rapidly oscillating function of k_1+k_2 (k_1 and k_2 being both positive k_1+k_2 cannot vanish)

- The second term becomes important when k_1-k_2 is close to zero (we have then $\delta_1-\delta_2=0$)

- Using:

$$\lim_{R\to\infty} \frac{1}{\pi} \frac{\sin \boldsymbol{R}\,\boldsymbol{x}}{\boldsymbol{x}} = \delta(\boldsymbol{x}) \tag{A.19}$$

we get:

$$\int_0^\infty \boldsymbol{u}_{k_1 l}(\boldsymbol{r})\, \boldsymbol{u}_{k_2 l}(\boldsymbol{r})\, \mathrm{d}\boldsymbol{r} = \frac{\pi}{2}\,\delta(\boldsymbol{k}_1 - \boldsymbol{k}_2) \tag{A.20}$$

- We then have, according to (A.2):

$$\int \mathrm{d}^3\boldsymbol{r}\; \varphi^*_{k'l'm'}(\vec{\boldsymbol{r}})\; \varphi_{klm}(\vec{\boldsymbol{r}}) = \frac{2}{\pi} \underbrace{\int \mathrm{d}\Omega\, \boldsymbol{Y}^*_{l'm'}(\theta,\varphi)\, \boldsymbol{Y}_{lm}(\theta,\varphi)}_{=\delta_{ll'}\delta_{mm'}} \underbrace{\int \boldsymbol{u}_{kl}(\boldsymbol{r})\, \boldsymbol{u}_{k'l}(\boldsymbol{r})\, \mathrm{d}\boldsymbol{r}}_{=\frac{\pi}{2}\delta(\boldsymbol{k}-\boldsymbol{k}')}$$

$$= \delta(\boldsymbol{k} - \boldsymbol{k}')\,\delta_{ll'}\delta_{mm'} \tag{A.21}$$

which demonstrates (A.1).

Demonstration of (A.8)

Let us apply E-H to the right side of (A.8). Using (A.10) and:

$$H = -\frac{\hbar^2}{2\mu}\Delta + V(r) = -\frac{\hbar^2}{2\mu}\left[\frac{1}{r}\frac{\partial^2}{\partial r^2} - \frac{\vec{L}^2}{\hbar^2 r^2} - \frac{2\mu}{\hbar^2}V(r)\right] \qquad \textbf{(A.22)}$$

we get, using (A.12):

$$\left(E - H\right)G^{(\pm)}\left(\vec{r},\vec{r}'\right) = -\frac{1}{krr'}\sum_{lm}\exp\left(\pm i\,\delta_l\right)Y^*_{lm}(\theta,\varphi)Y_{lm}(\theta',\varphi') \times$$

$$\times\left\{\left(F(r) + \frac{\partial^2}{\partial r^2}\right)\left[\theta\left(r - r'\right)u_{kl}(r')u^{\pm}_{kl}(r) + \theta\left(r' - r\right)u_{kl}(r)u^{\pm}_{kl}(r')\right]\right\} \qquad \textbf{(A.23)}$$

To calculate the second line of (A.23), we use:

$$\frac{\partial}{\partial r_1}\theta\left(r_1 - r_2\right) = -\frac{\partial}{\partial r_1}\theta\left(r_2 - r_1\right) = \delta\left(r_1 - r_2\right)$$

$$\left[\frac{\partial}{\partial r_1}\delta\left(r_1 - r_2\right)\right]f(r_1) = -f'(r_2)\delta\left(r_1 - r_2\right) + f(r_2)\left[\frac{\partial}{\partial r_1}\delta\left(r_1 - r_2\right)\right] \qquad \textbf{(A.24)}$$

The second order derivative of the second line of (A.23) gives 3 types of terms: proportional to $\theta(r - r')$ and $\theta(r' - r)$, to $\delta(r - r')$ and to $\partial\delta(r - r')/\partial r$

- The terms $\propto \theta(\boldsymbol{r} - \boldsymbol{r}')$ are multiplied by $\left[\boldsymbol{F}(\boldsymbol{r}) + \left(\partial^2 / \partial \boldsymbol{r}^2\right)\right] \boldsymbol{u}_{kl}^{\pm}(\boldsymbol{r})$ which vanishes because $\boldsymbol{u}_{kl}^{\pm}(\boldsymbol{r})$ is a solution of (A.3).
The same argument applies for the terms $\propto \theta(\boldsymbol{r}' - \boldsymbol{r})$ which are multiplied by $\left[\boldsymbol{F}(\boldsymbol{r}) + \left(\partial^2 / \partial \boldsymbol{r}^2\right)\right] \boldsymbol{u}_{kl}(\boldsymbol{r}) = 0$

- The terms proportional to $\partial \delta(\boldsymbol{r} - \boldsymbol{r}') / \partial \boldsymbol{r}$ cancel out

- The only terms surviving in the second line of (A.23) are those proportional to $\delta(\boldsymbol{r} - \boldsymbol{r}')$, which gives for this line:

$$\left[\boldsymbol{u}_{kl}(\boldsymbol{r}')\left(\partial \boldsymbol{u}_{kl}^{\pm}(\boldsymbol{r}') / \partial \boldsymbol{r}'\right) - \boldsymbol{u}_{kl}^{\pm}(\boldsymbol{r}')\left(\partial \boldsymbol{u}_{kl}(\boldsymbol{r}') / \partial \boldsymbol{r}'\right)\right] \delta(\boldsymbol{r} - \boldsymbol{r}') \qquad \textbf{(A.25)}$$

- We recognize in the bracket of (A.25) the Wronskian of $\boldsymbol{u}_{kl}$ and $\boldsymbol{u}_{kl}^{\pm}$
We can thus use (A.14) with $\boldsymbol{F}_1 = \boldsymbol{F}_2$ since $\boldsymbol{u}_{kl}$ and $\boldsymbol{u}_{kl}^{\pm}$ correspond to the same value of $\boldsymbol{k}$.

- Equation (A.14) shows that the Wronskian is independant of $\boldsymbol{r}$ when $\boldsymbol{F}_1 = \boldsymbol{F}_2$. We can thus calculate it for very large values of $\boldsymbol{r}$ where we know the asymptotic behavior (A.5) and (A.6) of $\boldsymbol{u}_{kl}$ and $\boldsymbol{u}_{kl}^{\pm}$

- The calculation of the Wronskian appearing in (A.25) is straightforward using (A.5) and (A.6) and gives:

$$W(u_{kl}, u_{kl}^{+}) = -k \exp(\mp i\delta_l) \tag{A.26}$$

- Inserting (A.26) into (A.25) and then in (A.23) gives:

$$(E - H) G^{(\pm)}(\vec{r}, \vec{r}') = \frac{1}{r^2}\delta(r - r')\sum_{lm} Y_{lm}^{*}(\theta, \varphi) Y_{lm}(\theta', \varphi') \tag{A.27}$$

- We can then use the closure relation for the spherical harmonics (see Ref. 3, Complement AVI):

$$\sum_{lm} Y_{lm}^{*}(\theta, \varphi) Y_{lm}(\theta', \varphi') = \delta(\cos\theta - \cos\theta')\,\delta(\varphi - \varphi') \tag{A.28}$$

to obtain:

$$\begin{aligned}(E - H) G^{(\pm)}(\vec{r}, \vec{r}') &= \frac{1}{r^2}\delta(r - r')\,\delta(\cos\theta - \cos\theta')\,\delta(\varphi - \varphi') \\ &= \delta(\vec{r} - \vec{r}')\end{aligned} \tag{A.29}$$

which demonstrates (A.8).

Asymptotic behavior of G⁺

For r very large, only the first term of the bracket of (A.10) is non zero and we get:

$$G^{(+)}(\vec{r},\vec{r}') \underset{r\to\infty}{\simeq} -\frac{2\mu}{\hbar^2}\frac{1}{krr'}\sum_{lm} e^{i\delta_l}\, Y^*_{lm}(\theta,\varphi)Y_{lm}(\theta',\varphi')u_{kl}(r')u^+_{kl}(r) \quad \text{(A.30)}$$

According to (A.6), we have

$$G^{(+)}(\vec{r},\vec{r}') \underset{r\to\infty}{\simeq} -\frac{2\mu}{\hbar^2}\frac{1}{kr'}\sum_{lm} (-i)^l e^{i\delta_l}\, Y^*_{lm}(\theta,\varphi)Y_{lm}(\theta',\varphi')u_{kl}(r')\frac{e^{ikr}}{r} \quad \text{(A.31)}$$

On the other hand, from Eq. (1.46) of lecture 1 and (A.2), we have:

$$\varphi^-_{k\vec{n}}(\vec{r}') = \frac{1}{k}\sqrt{\frac{2}{\pi}}\sum_{lm}(i)^l \exp(-i\delta_l)\, Y_{lm}^*(\vec{n})\, Y_{lm}(\vec{n}')\frac{u_{kl}(r')}{r'} \qquad \vec{n} = \frac{\vec{r}}{r} \quad \vec{n}' = \frac{\vec{r}'}{r'} \quad \text{(A.32)}$$

Using (A.32), we can rewrite (A.31) as:

$$G^{(+)}(\vec{r},\vec{r}') \underset{r\to\infty}{\simeq} -\frac{2\mu}{\hbar^2}\sqrt{\frac{\pi}{2}}\left[\varphi^-_{k\vec{n}}(\vec{r}')\right]^*\frac{e^{ikr}}{r} \quad \text{(A.33)}$$

which demonstrates Eq. (2.39) of lecture 2.