Notes from Ch. 11 (Taylor) & OSU

The Free Radial wave functions

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + p^2\right]\psi_{l,p}(r) = 0, \qquad \left(p = \frac{2mE}{\hbar^2}\right)$$

2nd order, Linear ODE
$\Rightarrow$ 2 solutions (L.I)
of these solutions:
The physically relevant $\rightarrow 0$ at $r=0$

Note:
as $r \rightarrow 0$ the centrifugal term dominates p^2

$\therefore$ the solutions behave like solutions of

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right)\psi(r) = 0$$

The combinations of r^{l+1} and r^{-l}
Thus the physically acceptable wavefunction is uniquelly determined as the one behaving like

$r^{l+1} \rightsquigarrow$ The Riccati-Bessel function

$$\boxed{\hat{j}_l(z) \equiv \left(\frac{\pi z}{2}\right) J_{l+\frac{1}{2}}(z)}$$

TABLE 11.1. RICCATI FUNCTIONS

	$l=0$	$l=1$	$l=2$
$\hat{j}_l(z)$	$\sin z$	$\frac{1}{z}\sin z - \cos z$	$\left(\frac{3}{z^2}-1\right)\sin z - \frac{3}{z}\cos z$
$\hat{n}_l(z)$	$\cos z$	$\frac{1}{z}\cos z + \sin z$	$\left(\frac{3}{z^2}-1\right)\cos z + \frac{3}{z}\sin z$
$\hat{h}_l^+(z)$	e^{iz}	$\left(1+\frac{i}{z}\right)e^{i(z-\pi/2)}$	$\left(1+\frac{3i}{z}-\frac{3}{z^2}\right)e^{i(z-\pi)}$
$\hat{h}_l^-(z)$	e^{-iz}	$\left(1-\frac{i}{z}\right)e^{-i(z-\pi/2)}$	$\left(1-\frac{3i}{z}-\frac{3}{z^2}\right)e^{-i(z-\pi)}$

Table 11.1 shows (as can be checked directly from the definitions) that the following useful identities hold:

$$\hat{j}_l(-z) = (-)^{l+1}\hat{j}_l(z)$$
$$\hat{n}_l(-z) = (-)^l\hat{n}_l(z)$$
$$\hat{h}_l^{\pm}(-z) = (-)^l\hat{h}_l^{\mp}(z)$$

Also, for real arguments $\hat{j}_l(x)$ and $\hat{n}_l(x)$ are real, whereas

$$[\hat{h}_l^{\pm}(x)]^* = \hat{h}_l^{\mp}(x) \qquad [x \text{ real}]$$

where if $[z \rightarrow \infty$, real$]$

$\hat{j}_l(z) = \sin(z - \frac{1}{2}l\pi) + O(z^{-1})$

with a similar result for

$\hat{n}_l(z) = \cos(z - \frac{1}{2}l\pi) + O(z^{-1})$

Partial waves — (NON free)

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - U(r) + p^2\right]\psi_{l,p}(r) = 0$$

As $r \rightarrow \infty$ $\psi_{l,p}(r)$ relates to $f_l(p)$ or $\delta_l(p)$

normalised radial wave function

BC: $\psi_{l,p}(0) = 0$

where $U(r) = 2m V(r)$

Integrating outward from $r=0$

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - U(r) + p^2\right]\psi_{l,p}(r) = 0$$

with $\psi_{l,p}(0)=0$ and with any convenient normalisation.

The solution $\propto \psi_{l,p}(r)$

At $r\to\infty$:

The solution behaves as $C \times \sin(pr - \frac{1}{2}l\pi + \delta_l)$, C is constant

Thus we need to integrate to $R_{max} \gg r^*$
(a point well beyond the influence of the potential)
and compare the resulting phase with:
$\sin(pr - \frac{1}{2}l\pi)$ (free wave function)

recall

$$\boxed{\hat{j}_l(z) \equiv \left(\frac{\pi z}{2}\right) J_{l+\frac{1}{2}}(z)}$$

where if [$z\to\infty$, real]
$\hat{j}_l(z) = \sin(z - \frac{1}{2}\pi) + O(z^{-1})$
with a similar result for
$\hat{n}_l(z) = \cos(z - \frac{1}{2}\pi) + O(z^{-1})$

We can completely divorce this framework from the 3D analysis (in which it was originated)

— Properties of the partial wave amplitude —

from
$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \lambda U(r) + p^2\right]\psi_{l,p}(r) = 0 \qquad (1)$$

we obtain $\psi_{l,p}(r)$ and from it we obtain

and $f_l(p) = \dfrac{e^{i\delta_l(p)}}{p}\sin\delta$ $\qquad \delta_l(p)$

- we introduced a strength parameter λ
- we assume (as usual) that $V(r)$ satisfies:
  1. $V(r) = O(r^{-3-\epsilon})$ as $r\to\infty$
  2. $V(r) = O(r^{-\frac{3}{2}+\epsilon})$ as $r\to 0$
  3. $V(r)$ is continuous for $0<r<\infty$ (except perhaps at a finite number of finite discontinuities)

Remarks

- if $\lambda U(r) \ll \frac{l(l+1)}{r^2} - p^2 \quad \forall r \Rightarrow$ (1) is a free radial equation
  then we would expect $\psi_{l,p}(r) \to \hat{j}_l(pr)$ and hence $f_l(p)\to 0$

as $\lambda\to 0$ (weaker potential) $f_l(p)\to 0$
and $\delta_l(p)\to n\pi$

.. Similarly at high energies $\to f_l(p)\to 0$ and $\delta_l(p)\to n\pi$
This is ambiguous
Therefore we can impose

$\delta_l(p)$ to be a continuous function that goes to zero as $p \to \infty$, furthermore, if this is done Then it is also zero as $\lambda \to 0$

As $l \to \infty$ (for a given potential and energy) we have the same results

$$f_l(p) \to 0 \quad \text{and} \quad \delta_l(p) \to n\pi$$

we understand this result by regarding $\frac{l(l+1)}{2mr^2}$ as a repulsive centrifugal potential the larger "l" the more repulsion due to the barrier and the smaller the chance that the incident particle will penetrate the region where $V(r)$ is appreciable.

This provides us with an estimate of l_{max} for which $\delta_l(p)$ is appreciable.

> See notes in page (105 in pdf) for info on the relevance of
>
> - The Born approximation.
> - Levinson's Theorem
> - Scattering crosssection

The regular solution $\phi(r) = u(r)$

Mathematically is convenient to discuss a solution that is defined by BCS at a single point.

$$\boxed{\phi_{l,p}(r) \xrightarrow[r \to 0]{} \hat{j}_l(pr)}$$

This requires:

$\phi_{l,p}(r)$ vanishes at $r=0$

VPA

Basics of VPA for $l=0$ case

1. we introduce $V_p(r) = \begin{cases} V_{Xe}(r) & r \le p \\ 0 & r > p \end{cases}$

@ $E = \frac{k^2}{2\mu}$ phase shifts

2. we denote the solution for $V_{Xe}(r)$ by $\phi(r)$ and the solution for $V_p(r)$ by $\phi_{l,p}(r)$

$\Rightarrow \begin{cases} V(r) : \delta \\ V_p(r) : \delta(p) \end{cases}$

3. we define $\boxed{\delta(0)=0}$ $\rightarrow r > \rho$: No potential $\Rightarrow$ No phase shift.

$* \; \phi_p(r) \equiv \phi(r)$ $[0 \le r \le p]$

we set up an ODE for $\delta(p)$ and integrate from $\rho = 0$ to $\rho \to \infty$

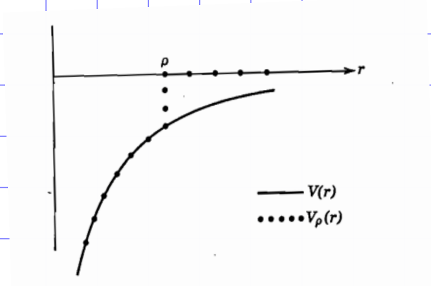


FIGURE 11.4. The truncated potential $V_p(r)$.

when $r > \rho$: $V_p(r) = 0$

$\therefore \delta(k, 0) = 0$

At $r \le \rho$ (large ρ)

AKA: The accumulation of phase shift

$V_p(r) = V_{Xe}(r)$

$\therefore \delta(k, \rho) \xrightarrow[\rho \to \infty]{} \delta(k)$

Then for fixed k the r-dependent phase shift satisfies

$$\frac{d}{dr}\delta(k,r) = -\frac{1}{k} U(r) \sin^2[kr + \delta(k,r)]$$

where $U(r) \equiv \frac{2\mu V(r)}{\hbar^2}$

as $r \to 0$

$$\frac{d}{dr}\delta(k,r) = -\frac{1}{k} U(r) \sin^2[kr] \quad (31)$$

$*$ An attractive potential $\Rightarrow \delta(k,r)$ increases positively

$\Rightarrow V(r) \le 0 \rightsquigarrow \delta(r) \ge 0$

For $l \neq 0$, solve equation

$$\frac{d}{dr}\delta_l(k,r) = -\frac{1}{k} U(r) \left[\cos(\delta_l(k,r)) \hat{j}_l(kr) - \sin(\delta_l(k,r)) \hat{n}_l(kr)\right]^2 \quad (32)$$

(Recall that $\hat{j}_0(z) = \sin z$ and $\hat{n}_0(z) = -\cos z$.) At a given point r_1, Eq. (25) has two unknowns, $\cos \delta_l$ and $\sin \delta_l$, so we need two equations to work with. Two ways to get them and extract δ_l are:

1. calculate at two different points $u(r_1)$ and $u(r_2)$, form $u(r_1)/u(r_2)$ and then solve for $\tan \delta(k)$;
2. calculate $u(r_1)$ and $u'(r_1)$, take the ratio and then solve for $\tan \delta$.

Either way works fine numerically if you have a good differential equation solver (for which you can specify error tolerances).

in general ($l \neq 0$)

Integrate δ' from $r=0$ to ($R_{max} << r$) asymptotic region with IC. $\delta(k,0) = 0$

$\therefore U_l(r) \xrightarrow[r \to \infty]{} \cos(\delta_l(k,r)) \hat{j}(kr) - \sin(\delta_l(k,r)) \hat{n}_l(kr)$

Nominally { we solve for δ by integrating the Schrödinger equation numerically in r from the origin (using any normalisation)
In response to the potential, the wave function is either pulled in (with each step in r) if $V(r)$ is attractive or pushed out (otherwise
This must be taken into account during integration

regular solution : $\phi(r)$ $\left(R = \frac{u_\ell(r)}{r} \right)$

2D radial Schrödinger equation $(\ell = 0)$

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

where $E = \frac{k^2\hbar^2}{2\mu}$ $\therefore -k^2 = \frac{-2\mu E}{\hbar^2}$

$$-k^2 u(r) = \frac{d^2 u(r)}{dr^2} + \frac{u(r)}{4r^2} - \frac{2\mu V(r)\,u(r)}{\hbar^2} \qquad (2)$$

$$\therefore 0 = \frac{u''}{u} + k^2 + \frac{1}{4r^2} - \frac{2\mu V(r)}{\hbar^2} \qquad (3)$$

By (37) in OSU

$$* \quad \frac{d}{dr}\left(\frac{u'}{u}\right) = \frac{u''}{u} - \left(\frac{u'}{u}\right)^2 \qquad \therefore \frac{u''}{u} = -\frac{1}{4r^2} - \left(k^2 - \frac{2\mu}{\hbar^2}V(r)\right)$$

Hypothesis $\begin{cases} V_{Xe}(r) \text{ reproduces X-electron} \\ (\ell=0) \text{ S-wave phase shifts (symmetric)} \end{cases}$

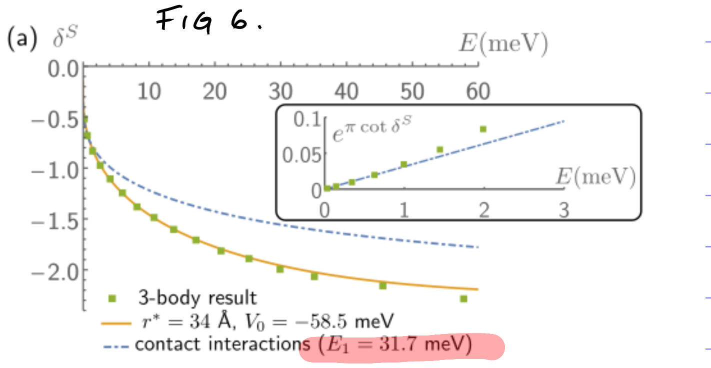
$$V_{X_e}(r) = \begin{cases} V_0 & r < r^* \\ -\frac{\alpha}{2}\left(\frac{dV_i(r)}{dr}\right)^2 & r > r^* \end{cases}$$

Table II (MoS_2, symmetric case)

V_0 (meV)	−58.5
r^* (Å)	34
α (10^3 au)	52

Energy range : $0 < E < 60$ meV

FIG 6.



– Integrate a System of ODEs –

scipy.integrate.odeint($\underbrace{\text{func}}$, $\underbrace{y_0}_{\text{IC(s)}}$, $\underbrace{t}_{\text{monotone sequence}}$, $\underbrace{\text{args}=()}_{\text{extra arguments}}$, $\overbrace{\text{Dfun=None}}^{\text{Jacobian of funct}}$, col_deriv=0,

if Dfun then derivatives: columns

full_output=0, ~~ml=None~~, ~~mu=None~~, ~~rtol=None~~, ~~tcrit=None~~, ~~h0=0.0~~,

return dictionary

~~hmax=0.0~~, ~~hmin=0.0~~, ~~ixpr=0~~, ~~mxstep=0~~, ~~mxhnil=0~~, ~~mxordn=12~~,

prints msg of convergence

mxords=5, printmessg=0, tfirst=False)

X: other optional param.

dy/dt = func(y, t, ...) or [funct(t, y, ...)]

where • y can be a vector.

must set to True if funct(t, y, ...)

return y: array shape (len(t), ~~len(y₀)~~)

$N = \text{len}(r)$

we want a large r

```python
def ODE_32(r, delta, k, l):
    # Set l != 0 manually for higher energy scattering
    top = -(2 * M_red * V_Xe(r) / (hbar**2)) * (np.cos(delta) * riccati_jn(l, k * r)[0][l] - np.sin(delta) * riccati_yn(l, k * r)[0][l])**2
    ddelta_dr = top / k
    return ddelta_dr

# ODE solver ODEINT
delta = []
for i, k_i in enumerate(k):
    # print(i)
    l = 0
    solution_ODE = odeint(
                    lambda r, delta : ODE_32(r, delta, k_i, l),
                    delta_0, r, tfirst=True
                    )
    delta.append(solution_ODE[-1] - np.pi)
```

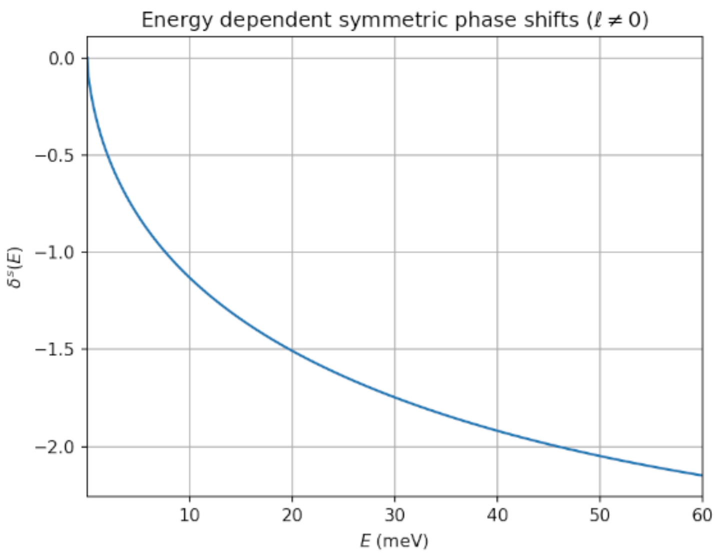
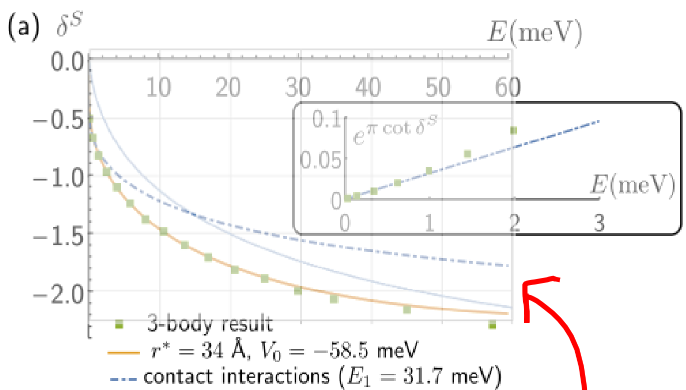


Fig 1. phase shift plot

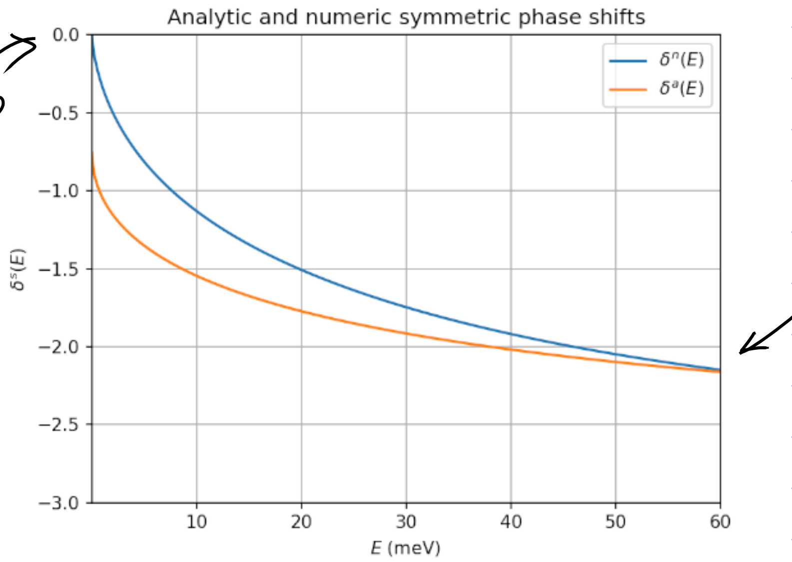


Is this converged with respect to how large r is?

Disagreement with Schmidt.

BUG What is wrong with my numerical result?

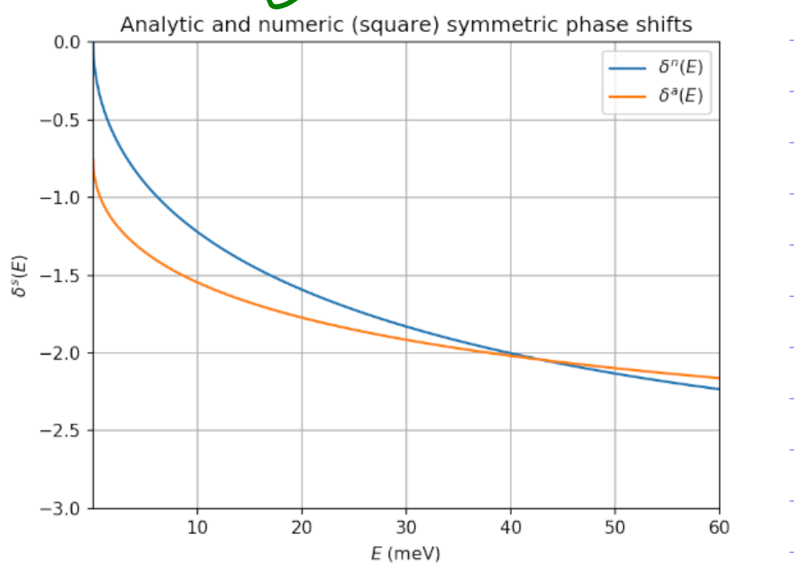
zero?



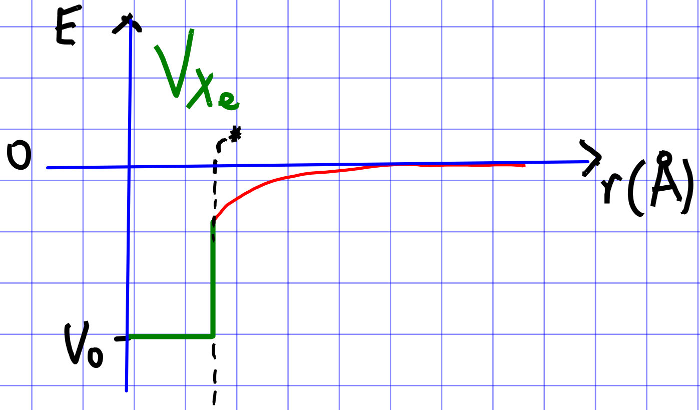
agreement at high energies. WHY?

$\mathrm{ODE\_32}(r, \delta, \kappa, l=0) = \mathrm{ODE\_31}(r, \delta, \kappa) = \frac{-2\mu V_{xe}(r)}{k\hbar^2} \sin^2(kr+\delta)$

Test using square well



– Jesper's Question –



- analytically solve:

$$\delta' = \frac{-2\mu V_{Xe}(r^*)}{\hbar^2 k}\left[\cos(\delta)\hat{j}_l(kr) - \sin(\delta)\hat{n}_l(kr)\right]^2 ?$$

where $V_{Xe}(r^*) = V_0 = -58.5\,\text{meV}$

⤳ work out how much phase a constant potential contributes.

The free state energy: $E_{tot} = \frac{\hbar^2 k_{free}^2}{2\mu} = K$

$(V(r) = 0)$

plane wave: $\psi(r) = e^{ikr} = e^{i\delta}$

(k is wave number)

$\therefore \delta = kr$

when $V(r) \neq 0$:

$$E_{tot} = K + V(r)$$

$$E_{tot} = \frac{\hbar^2 k_{eff}^2}{2\mu} + V$$

$$\frac{\hbar^2 k_{eff}^2}{2\mu} = E_{tot} - V$$

if $V = V_0$

$$\therefore \frac{\hbar^2 k_{eff}^2}{2\mu} = E - V_0 = \frac{\hbar^2 k_{free}^2}{2\mu} - V_0$$

$$\therefore k_{eff}^2 = k_{free}^2 - \frac{2\mu V_0}{\hbar^2}$$

then: $k_{eff} = \sqrt{k_{free}^2 - \frac{2\mu V_0}{\hbar^2}}$

$$\therefore \delta_0(r) = k_{eff}\, r^* = r^* \sqrt{k_{free}^2 - \frac{2\mu V_0}{\hbar^2}}$$

We want to use this to verify our numerical results for the (VPA):

$$⤳\ \delta_{VPA}(r) = k_{VPA}\, r$$

where $k_{VPA} = k_{eff} - k_{free}$ ⤳ since (VPA) results in the accumulated phase due to a potential (only)

$$\therefore k_{VPA} = \sqrt{k_{free}^2 - \frac{2\mu V_0}{\hbar^2}} - k_{free} = k_{free}\left(\sqrt{1 - \frac{2\mu V_0}{\hbar^2}} - 1\right)$$

$$\boxed{\therefore \delta_{VPA}(r) = k_{VPA}\, r = k_{free}\left(\sqrt{1 - \frac{2\mu V_0}{\hbar^2 k_{free}^2}} - 1\right) r}$$

in code $r = r^*$

Derivation Analytic Phase shift
(For square well in 2D)

$* E(k) = \frac{\hbar^2 k^2}{2\mu}$

Bug $\oslash$SU(32) solver

Aw look how cute

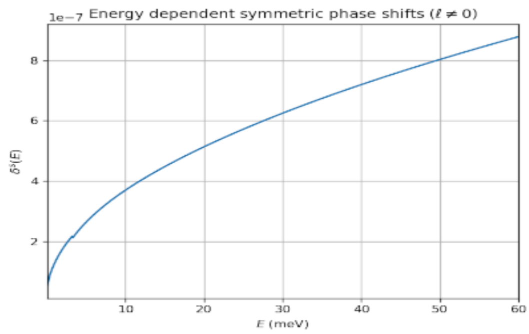
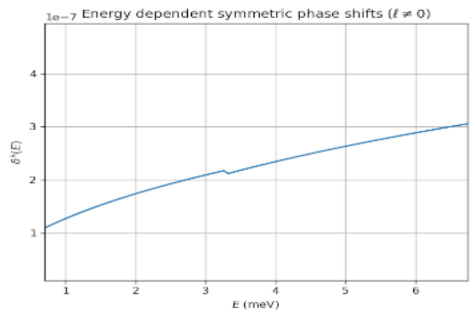


FIG.2
Enhance!



if $E = \frac{\hbar^2 k^2}{2\mu}$ where $E \in [1e\text{-}6, 60]$ meV

To use eqn(32) and (31)

I need: $\therefore k = \sqrt{\frac{2\mu E}{\hbar^2}}$ $\left[\frac{rad}{m}\right]$

IC: $\delta(0) = 0$

ODE (31) $\rightsquigarrow$ $\frac{-U(r)\sin^2(kr+\delta)}{k} = \delta'$

$\left[\frac{rad}{m}\right]^2 \left[\frac{m}{rad}\right] = \left[\frac{rad}{m}\right]$

in Taylor $U(r) = \frac{2\mu V_{Xe}(r)}{\hbar^2}$ $\left[\frac{rad^2}{m^2}\right]$ Potential in (wave number units)^2

In SI units

$V_0 = -58.5$ meV $= -9.37e\text{-}21$ [J]

$V_{Xe} \begin{cases} V_0 \\ -\frac{\alpha}{2} q^2 \left(\frac{dV_k(r)}{dr}\right)^2 \end{cases}$

$\therefore$ ODE:

```
ana@ana-XPS-13-9343:~/scatterbrain$ python3 TESTING_scatterbrain.py
M_red=2.921773226981081e-31   [kg]

V_Xe(r)=array([-9.37273331e-21, -9.37273331e-21, -9.37273331e-21, ...,   [J]
       -4.54335706e-24, -4.52700972e-24, -4.51073541e-24])

hbar**2=1.11212168135524e-68   [Js]^2   [1e-6,20

k=array([9.17523705e+04, 2.22207545e+07, 3.14247584e+07, ...,
       7.10015734e+08, 7.10363355e+08, 7.10710806e+08])

r=array([1.00000000e-16, 1.95504420e-11, 3.91007841e-11, ...,   [m]
       1.99608993e-08, 1.99804497e-08, 2.00000000e-08])

k * r=array([9.17523705e-12, 4.34425572e-04, 1.22873269e-03, ...,
       1.41725526e+01, 1.41933793e+01, 1.42142161e+01])

This is the accumulation of phase shift: [8.790641e-07]
ana@ana-XPS-13-9343:~/scatterbrain$
```

$q = e^-$ [C] $\therefore q^2 = 2.56e\text{-}38 [C^2]$

$V_k = \left[\frac{J}{C^2}\right]$ $\therefore \left(\frac{dV_k(r)}{dr}\right)^2 = \left[\frac{N^2 m^2}{C^4}\right]\left[\frac{1}{m^2}\right] = \left[\frac{N^2}{C^4}\right]$

$\alpha = 8.57e^{-37} [C^2 m^2 J^{-1}]$

$\left[\frac{\alpha}{2} q^2 \left(\frac{dV_k(r)}{r}\right)^2\right] = \left[\frac{C^2 m^2}{Nm}\right]\left[C^2\right]\left[\frac{N^2}{C^4}\right] = [J]$

fix: delta.append(solution_ODE[$\cancel{1}$]) index should be -1

Largest k in array given $0 \leq E \leq 60$ meV

$$k_{max} = \sqrt{\frac{2\mu V_0}{\hbar^2}} \approx 7.10e8$$

wavelength $\lambda = \frac{2\pi}{Å}$

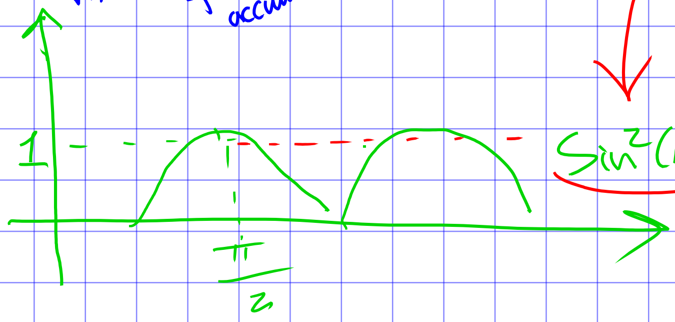
$\delta(0) = 0$

$k \to \infty$

$\delta(k) >> \delta(0)$

$\lambda = \frac{2\pi \, [rad]}{3441747 \, [\frac{rad}{m}]}$ ← rate of phase accumulation

we want δ' large



$\sin^2(kr + \delta)$

we want $r * k = \frac{\pi}{2}$

where $r < r^*$

$kr = \frac{\pi}{2}$

$\therefore k = \frac{\pi}{2} 10^{10}$

$$\frac{1 rad}{Å} = \frac{1 rad}{10^{-10}} = 1 rad \times 10^{10}$$

if $r^* = 34Å$

Are my k's too small?

— My r was too small —