# Friedel Oscillations

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## 1　问题

动量空间中电势为

$$\varphi(\vec{q}) = \frac{\varphi_{ext(\vec{q})}}{\varepsilon(\vec{q})} \tag{1}$$

其中

$$\varphi_{ext}(\vec{q}) = \frac{-e}{\varepsilon_0 V q^2} \tag{2}$$

所以

$$\varphi(\vec{q}) = \frac{-e}{\varepsilon_0 V q^2 \varepsilon(\vec{q})} \tag{3}$$

### 1.1　Thomas-Fermi 近似的结果

Thomas-Fermi 近似给出

$$\varepsilon_{TF}(\vec{q}) = 1 + \frac{q_{TF}^2}{q^2} \tag{4}$$

将上式代入 $\varphi(\vec{q})$ 有

$$\varphi(\vec{q}) = \frac{-e}{\varepsilon_0 V q^2 \left(1 + \frac{q_{TF}^2}{q^2}\right)} = \frac{-e}{\varepsilon_0 V \left(q^2 + q_{TF}^2\right)} \tag{5}$$

对其 Fourier Transform

$$\varphi(\vec{r}) = \int_{-\infty}^{+\infty} e^{i\vec{q}\cdot\vec{r}}\varphi(\vec{q})\mathrm{d}^3q \tag{6}$$

$$= \frac{-e}{2\pi^2\varepsilon_0}\cdot\frac{1}{r}\int_0^{+\infty}\sin(qr)\cdot\frac{q}{q^2+q_{TF}^2}\mathrm{d}q \tag{7}$$

$$= \frac{-e}{4\pi\varepsilon_0}\cdot\frac{1}{r}\cdot\frac{\pi}{2}\int_0^{+\infty}\sin(qr)\cdot\frac{q}{q^2+q_{TF}^2}\mathrm{d}q \tag{8}$$

对 $\frac{q}{q^2+q_{TF}^2}$ 在 $q\to+\infty$ 展开 (与在 $q_{TF}\to 0$ 时对 $q_{TF}$ 展开相同):

```
In [61]: import sympy as sym
         q = sym.Symbol('q')
         q_tf = sym.Symbol('q_TF')
         s = sym.series(q/(q**2+q_tf**2),q,sym.oo,5)
         print(sym.latex(s))
```

```
- \frac{q_{TF}^{2}}{q^{3}} + \frac{1}{q} + O\left(\frac{1}{q^{5}}; q\rightarrow \infty\right)
```

$$\frac{q}{q^2+q_{TF}^2} = \frac{q_{TF}^2}{q^3}+\frac{1}{q}+O\left(\frac{1}{q^5};q\to\infty\right) \tag{9}$$

计算 leading order

$$\int_0^{+\infty}\sin(qr)\cdot\frac{1}{q}\mathrm{d}q = \frac{1}{2i}\int_{-\infty}^{+\infty}e^{iqr}\cdot\frac{1}{q}\mathrm{d}q = \frac{1}{2i}\cdot\pi i\cdot 1 = \frac{\pi}{2} \tag{10}$$

这正好是精确结果

$$\frac{-e}{4\pi\varepsilon_0}\cdot\frac{e^{-q_{TF}r}}{r} \tag{11}$$

在 $q_{TF}\to 0$ 时对 $q_{TF}$ 展开的结果的 leading order 相同.

问题 1: Thomas-Fermi 近似结果与精确结果的 $q_{TF}^2$ 的系数不同? 问题 2: 为什么要对 $q$ 在 $q\to+\infty$ 展开? 积分的区间不是整个实轴吗?

### 1.2 RPA 的结果

RPA 给出

$$\varepsilon(\vec{q}) = 1+\frac{q_{TF}^2}{q^2}g\left(\frac{q}{2k_F}\right) \tag{12}$$

将上式代入 ( ) 有

$$\varphi(\vec{q}) = \frac{-e}{\varepsilon_0 V q^2 \left(1+\frac{q_{TF}^2}{q^2}\right)} = \frac{-e}{\varepsilon_0 V \left(q^2 + q_{TF}^2 g\left(\frac{q}{2k_F}\right)\right)} \tag{13}$$

其中

$$g(u) = \frac{1}{2}\left(1 + \frac{1}{2u}(1-u^2)\ln\left|\frac{1+u}{1-u}\right|\right) \tag{14}$$

对 ( ) 作 Fourier Transform

$$\varphi(\vec{r}) = \frac{-e}{2\pi^2\varepsilon_0}\cdot\frac{1}{r}\int_0^{+\infty}\sin(qr)\cdot\frac{q}{q^2+q_{TF}^2 g(\frac{q}{2k_F})}\mathrm{d}q \tag{15}$$

### 1.2.1 级数展开

对 $\frac{q}{q^2+q_{TF}^2 g(\frac{q}{2k_F})}$ 在 $q\to+\infty$ 展开

```
In [60]: import sympy as sym
         q = sym.Symbol('q')
         q_tf = sym.Symbol('q_TF')
         kf = sym.Symbol('k_F')
         u = q/(2*kf)
         #g=1
         g = sym.Rational(1,2)*( 1+(1-u**2)/(2*u)*sym.log((u+1)/(u-1) ) )
         s = sym.series(q/(q**2+q_tf**2)*g,q,sym.oo,10)
         print(sym.latex(s))
```

```
\frac{\frac{256 k_{F}^{8}}{63} - \frac{64 k_{F}^{6} q_{TF}^{2}}{35} + \frac{16 k_{F}^{4} q_{TF
```

$$\frac{q}{q^2+q_{TF}^2 g(\frac{q}{2k_F})} = \frac{\frac{256k_F^8}{63} - \frac{64k_F^6 q_{TF}^2}{35} + \frac{16k_F^4 q_{TF}^4}{15}}{q^9} + \frac{\frac{64k_F^6}{35} - \frac{16k_F^4 q_{TF}^2}{15} + \frac{4k_F^2 q_{TF}^4}{3}}{q^7} + \frac{\frac{16k_F^4}{15} - \frac{4k_F^2 q_{TF}^2}{3}}{q^5} + \frac{4k_F^2}{3q^3} + O\left(\frac{1}{q^{10}}; q\to\infty\right) \tag{16}$$

问题 3: 接下来该怎么做? 所有的展开项代入积分都是发散的.

# 2 参考文献

Friedel Oscillation 的原始文献 the shielding of a fixed charge in a high-density electron gas http://www.doc88.com/p-9512851691956.html