Consider the electrostatic energy of a set of point charges \( Q_j \) at \( \vec{r}_j \):

\[
E_H = \frac{1}{2} \sum_{i \neq j} \frac{Q_i Q_j}{|\vec{r}_i - \vec{r}_j|}
\]

Due to the long range of \( \frac{1}{r} \) this sum can be ill-defined for \( \infty \) d or periodic systems (IR divergence). So we just cut off the Coulomb \( \frac{1}{r} \) potential at long distance \( r > \Lambda \) and call it \( v^\Lambda (r) \). Examples are:

\[
v^\Lambda (r) = e^{-r^\Lambda} \quad \text{Yukawa cutoff}
= \frac{erfc(r/\Lambda)}{r} \quad \text{Gaussian (Ewald) cutoff}
\]

We will later send \( \Lambda \to +\infty \) and see what happen.

So

\[
E_H^\Lambda = \frac{1}{2} \sum_{j \neq k} Q_j Q_k v^\Lambda (|\vec{r}_j - \vec{r}_k|)
\]

Notice that \( v^\Lambda (0) \) never occurs here so there is no short-ranged (UV) divergence possible.

To make some progress, we see that

\[
E_H^\Lambda = \frac{1}{2} \sum_j Q_j \phi_j, \quad \phi_j = \sum_k Q_k v^\Lambda (|\vec{r}_k - \vec{r}_j|)
\]
So the real challenge is to find $\phi_j$.

Elementary point: even if $\phi_j$ is well-defined, the sum over $j$ in $E^j = \frac{1}{2} \Sigma Q_j \phi_j$ may diverge simply because the number of charges is large as $n \to \infty$. So we really should just focus on $\phi_j$ since it is intensive + $\phi_j/2$ is energy per particle per unit charge.

$$\phi_j = \sum_{k \neq j} Q_k V^j(r_{kj}) \quad r_{kj} = \frac{\mathbf{r}_k - \mathbf{r}_j}{\|r_{kj}\|}$$

This sum converges for $\lambda > 0$ so we now find a good way to calculate it by splitting up $V^j$ into a short-ranged + long-ranged part a-la-Emald:

$$V^j(r) = V^1(r) + V^2(r) + V^3(r)$$

$$= V^2(r) + V^3(r)$$

where $\lambda \ll \lambda$ is a microscopic cutoff used for efficient computation. $\lambda$ is fixed.

$$\phi_j = \sum_{k \neq j} Q_k V^1(r_{kj}) + \sum_{k \neq j} Q_k V^2(r_{kj})$$

$\phi^1_j$ + $\phi^2_j$ is a rapidly convergent sum in real space. $\phi^3_j$ is not a worry.
\[ \phi_{j\ell} = \sum_k Q_k \nabla \cdot (r_{kj}) - Q_j \nabla \cdot (r) \]

where we added & subtracted \( j \) to restrict \( \ell \)-sum for Fourier analysis. We expect \( \nabla \cdot (r) \) to be finite as both \( \nabla \cdot \nabla \) behave as \( \frac{1}{r^2} + O(r^0) \) as \( r \to 0 \) as the difference should be finite. Examples:

**Yukawa case:** \( \nabla \cdot (r) = \lim_{r \to 0} \frac{r^{-\lambda} - r^{-\lambda'}}{r} = \frac{1}{\lambda} - \frac{1}{\lambda'} \)

**Gaussian case:** \( \nabla \cdot (r) = \lim_{r \to 0} \frac{\text{erfc}(\frac{\lambda}{r}) - \text{erfc}(\frac{\lambda'}{r})}{\sqrt{\pi}} = \frac{2}{\sqrt{\pi}} \left( \frac{1}{\lambda} - \frac{1}{\lambda'} \right) \)

Also, the appearance of \( \nabla \cdot (r) \) is in some sense artificial since it is canceled by the \( j=\ell \) term.

\[ \phi_{j\ell} = \sum_k Q_k \nabla \cdot (r_{kj}) - Q_j \nabla \cdot (r) \]

Now Fourier analyze \( \nu_{\ell}(r) = \int \frac{d^3 \beta}{(2\pi)^3} e^{i \frac{\hat{r} \cdot \hat{\beta}}{\beta}} \nabla \cdot (r_{kj}) \)

Examples:

- **Coulomb** \( \frac{1}{r} \to \frac{4\pi}{\beta^2} \)
- **Yukawa** \( e^{-r^\lambda} \to \frac{4\pi}{\beta^2 + \lambda^{-2}} \)
- **Gaussian** \( \text{erfc}(\frac{\lambda}{r}) \to \frac{4\pi}{\beta^2} \left( 1 - e^{-\beta^2} \right) \)

\[ \phi_{j\ell} = \int \frac{d^3 \beta}{(2\pi)^3} \nabla \cdot (r_{kj}) \sum_k Q_k e^{i \frac{\hat{r} \cdot \hat{\beta}}{\beta}} - Q_j \nabla \cdot (r) \]

\[ = \int \frac{d^3 \beta}{(2\pi)^3} \nabla \cdot (r_{kj}) e^{i \frac{\hat{r} \cdot \hat{\beta}}{\beta}} S(\frac{\hat{r}}{\beta}) - Q_j \nabla \cdot (r) \]

\[ S(\frac{\hat{r}}{\beta}) = \sum_k Q_k e^{i \frac{\hat{r} \cdot \hat{\beta}}{\beta}} \text{ structure factor} \]
The potentially troublesome part of the integral is around \( \delta \approx 0 \) where \( \hat{\psi}_k(0) \) can become large as \( \Lambda \to \infty \): e.g.,

\[
\hat{\psi}_k(0) = 4\pi \frac{4\pi}{\delta^2 + \Lambda^2} - \frac{4\pi}{\delta^2 + \lambda^2}
\]

\( \hat{\psi}_k(0) = 4\pi(\Lambda^2 - \lambda^2) \) for Yukawa

\( \hat{\psi}_k(0) = \pi(\Lambda^2 - \lambda^2) \) for Gaussian

But for a neutral system, \( \sum_{k} q_k = \sum_{k} q_k = 0 \),

\( \hat{\psi}_k(0) \) is not relevant. If \( S(0) \neq 0 \), we may get in trouble.

To be more precise, we will assume a periodic system:

- lattice vectors \( \mathbf{R} \), positions in unit cell are \( \mathbf{r} \).
- \( S(\mathbf{q}) = \sum_{\mathbf{R}} e^{i\mathbf{q}\cdot\mathbf{R}} \sum_{\mathbf{r}} e^{i\mathbf{q}\cdot\mathbf{r}} \)
- \( S(\mathbf{q}) = \sum_{\mathbf{r}} e^{i\mathbf{q}\cdot\mathbf{r}} \frac{1}{\Omega} \sum_{\mathbf{R}} \delta^{\mathbf{R}}(\mathbf{q} - \mathbf{G}) \)
- \( \Sigma = \text{volume of unit cell} \)

So

\[
\phi = \sum_{\mathbf{q}} \frac{-i\mathbf{q}}{\Omega} \hat{\psi}_k(0) \frac{\partial}{\partial \mathbf{q}} \left[ S(\mathbf{G}) - Q_\tau \hat{\psi}_k(0) \right]
\]

\[
\phi = \sum_{\mathbf{G} \neq 0} \frac{-i\mathbf{G}}{\Omega} \hat{\psi}_k(0) \frac{\partial}{\partial \mathbf{G}} \left[ S(\mathbf{G}) + \hat{\psi}_k(0) \right] \frac{\partial}{\partial \mathbf{G}} \left( S(0) - Q_\tau \hat{\psi}_k(0) \right)
\]

rapidly convergent for large \( \mathbf{G} \), since

\( \hat{\psi}_k(0) \to 0 \) faster than \( 1/\mathbf{G}^2 \) as \( |\mathbf{G}| \to \infty \)

\( \frac{1}{\mathbf{G}^2} \ll 1 \)
For periodic system we then have

\[
\psi = \sum_{R, \tau} Q_{\tau} \psi_{s}(||R+\frac{\tau}{2}-\frac{\tau}{2}||) + \sum_{G \neq 0} e^{i\frac{\pi}{2} v_{s}(G) s(G)} + \frac{\hat{v}_{s}(0) s(0)}{\Omega} - Q_{\tau} v_{s}(0)
\]

- the first 2 terms converge very well
- the third may be trouble
- the fourth is finite \( \lambda \) dependent

\[
v_{s}(0) \sim \frac{1}{\lambda} - \frac{1}{\lambda} \quad \text{is well-behaved for } \Lambda \to \infty
\]

\[
\hat{v}_{s}(0) \sim \Lambda^{2} - \lambda^{2} \quad \text{is divergent for } \Lambda \to \infty
\]

So we need \( s(0) = 0 = \sum_{\tau} Q_{\tau} \text{ nat. unit cell} \)

If \( s(0) \neq 0 \) answer is \( \infty \) and certainly depends on details of cutoff \( \Lambda \)

When \( \sum_{\tau} Q_{\tau} = 0 \), we can send \( \Lambda \to \infty \) and get a well-defined answer.

Final answer: \( \rightarrow \)
1. Let \( S(\vec{r}) = \sum_{n, \tau} Q_{\tau} e^{i \vec{\delta} \cdot \vec{r}} \), \( S(0) = 0 \) required.

2. Pick finite \( \lambda \) and define

\[
\psi_s(\vec{r}) = \nu^\lambda(\vec{r}) \\
\nu_\ell(\vec{r}) = \frac{1}{r} - \nu^\lambda(\vec{r}) \\
\nu_\ell(0) \sim 1/r
\]

3. Compute

\[
\phi_{\tau} = \sum_{n, \tau}^{\text{R, T}} Q_{\tau} \cdot \nu^\lambda(\vec{r} + \vec{e} - \vec{r}) + \sum_{\delta \neq 0} \frac{\hat{\psi}_\ell(\vec{r}) e^{-i \vec{\delta} \cdot \vec{r}}} {\Omega} S(\vec{r}) \\
- Q_{\tau} \nu_\ell(0)
\]

4. \( E_{\text{cell}} \) = \( \frac{1}{2} \sum_{\tau} Q_{\tau} \phi_{\tau} \)