

$$z_{n'}^{(1)}(\mathbf{k}_{\text{eff}}^+; n; \alpha) = -\frac{1}{\varepsilon_{\mathbf{k}_{\text{eff}}^+, n'}^{(0)} - \varepsilon_{\mathbf{k}, n}^{(0)}} \times \left\{ \left\langle \tilde{\psi}_{\mathbf{k}_{\text{eff}}^+, n'}^{(0)} \left| \mathcal{Z}_{\text{eff}}^{(1)}(q^+ \alpha) \right| \psi_{\mathbf{k}, n}^{(0)} \right\rangle_{\text{IR}} + \sum_{\gamma} \left\langle \tilde{\psi}_{\mathbf{k}_{\text{eff}}^+, n'}^{(0)} \left| \mathcal{Z}_{\text{eff}}^{(1)}(q^+ \alpha) + \nabla \mathcal{Z}_{\text{eff}}^{(0)} \delta_{\gamma \alpha} \right| \tilde{\psi}_{\mathbf{k}, n}^{(0)} \right\rangle_{\gamma} + \left\langle \tilde{\psi}_{\mathbf{k}_{\text{eff}}^+, n'}^{(0)} \left| \mathcal{Z}^{(0)} - \varepsilon_{\mathbf{k}, n}^{(0)} \right| \tilde{\psi}_{\mathbf{k}, n}^{(0)} \right\rangle_{\alpha} + \left\langle \tilde{\psi}_{\mathbf{k}_{\text{eff}}^+, n'}^{(0)} \left| \mathcal{Z}^{(0)} - \varepsilon_{\mathbf{k}, n}^{(0)} \right| \tilde{\psi}_{\mathbf{k}, n}^{(0)} \right\rangle_{\alpha} - \oint_{\partial \text{IR}_{\alpha}} \hat{\varepsilon}_{\text{IR}} \psi_{\mathbf{k}_{\text{eff}}^+, n'}^{*(0) \text{IR}} \left(\mathcal{Z}^{(0)} - \varepsilon_{\mathbf{k}, n}^{(0)} \right) \psi_{\mathbf{k}, n}^{(0) \text{IR}} dS \right\}$$

```

for l' = 0 to l_max, alpha do
  l'_Delta = 0.5 * l' * (l' + 1) ; // Triangular numbers
  for l = 0 to l' do
    l = l + l'_Delta ; // Packed storage for l', l
    for l'' = 0 to l_max, alpha do
      if l + l' + l'' even ^ |l - l'| < l'' < |l + l'| then // G_{l', l'', l}^{m', m'', m} finite
        for m'' <= |l''| do
          L'' = l'' * (l'' + 1) + 1 + m'' ; // Packed storage for l'', m''
          uvu[l, L''] = \sum_{l'l''m''}^{1\gamma} (q^+ \alpha);
          dvu[l, L''] = \sum_{l'l''m''}^{2\gamma} (q^+ \alpha);
          uvd[l, L''] = \sum_{l'l''m''}^{12\gamma} (q^+ \alpha);
          dvd[l, L''] = \sum_{l'l''m''}^{22\gamma} (q^+ \alpha);
        end for
      end if
    end for
  end for
end for
end for

```

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Density-Functional Perturbation Theory within the All-Electron Full-Potential Linearized Augmented Plane-Wave Method: Application to Phonons

Christian-Roman Gerhorst

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