Real-space Operation of Nonlocal Pseudopotentials

12/15/99

[R.D. King-Smith, M.C. Payne, and J.S. Lin, Phys. Rev. B44, 13063 ('91)]

— Kleinman-Bylander fully-nonlocal pseudopotential

$$\begin{cases} \hat{V}_{KB} = V^{PP}_{ion,local}(r) + V_{NL}(\mathbf{r},\mathbf{r}') & (1) \\ V_{NL}(\mathbf{r},\mathbf{r}') = \sum_{lm} \dfrac{Y_{lm}(\hat{r})\Delta V_l(r) R^{PP}_l(r)\; R^{PP}_l(r')\Delta V_l(r') Y^*_{lm}(\hat{r}')}{\langle R^{PP}_l | \Delta V_l | R^{PP}_l \rangle} & (2) \end{cases}$$

where

$$\langle R^{PP}_l | \Delta V_l | R^{PP}_l \rangle = \int dr\, r^2\, |R^{PP}_l(r)|^2 \Delta V_l(r) \tag{3}$$

$$\boxed{\begin{aligned} \hat{V}_{NL}|\psi\rangle &= \int d\mathbf{r}'\, V_{NL}(\mathbf{r},\mathbf{r}')\,\psi(\mathbf{r}') \\ &= \sum_{lm} \frac{Y_{lm}(\hat{r})\Delta V_l(r) R^{PP}_l(r)}{\langle R^{PP}_l | \Delta V_l | R^{PP}_l \rangle} \int d\mathbf{r}'\, R^{PP}_l(r')\Delta V_l(r') Y^*_{lm}(\hat{r}')\,\psi(\mathbf{r}') \end{aligned}} \quad (4)$$

※ Note that the $\mathbf{r}'$ integral is finite-ranged since $\Delta V_l(r') = 0$ for $r' \geq r_c = \max\{r_{cl}\}$.

- Operation count

for each orbital n

$\hat{V}_{NL}|\psi_n\rangle \leftarrow 0$

for each ion I

$A_l \leftarrow \int dr\, r^2 |R_l^{PP}(r)|^2 \Delta V_l(r) \quad (l = 0, \ldots, l_{max})$

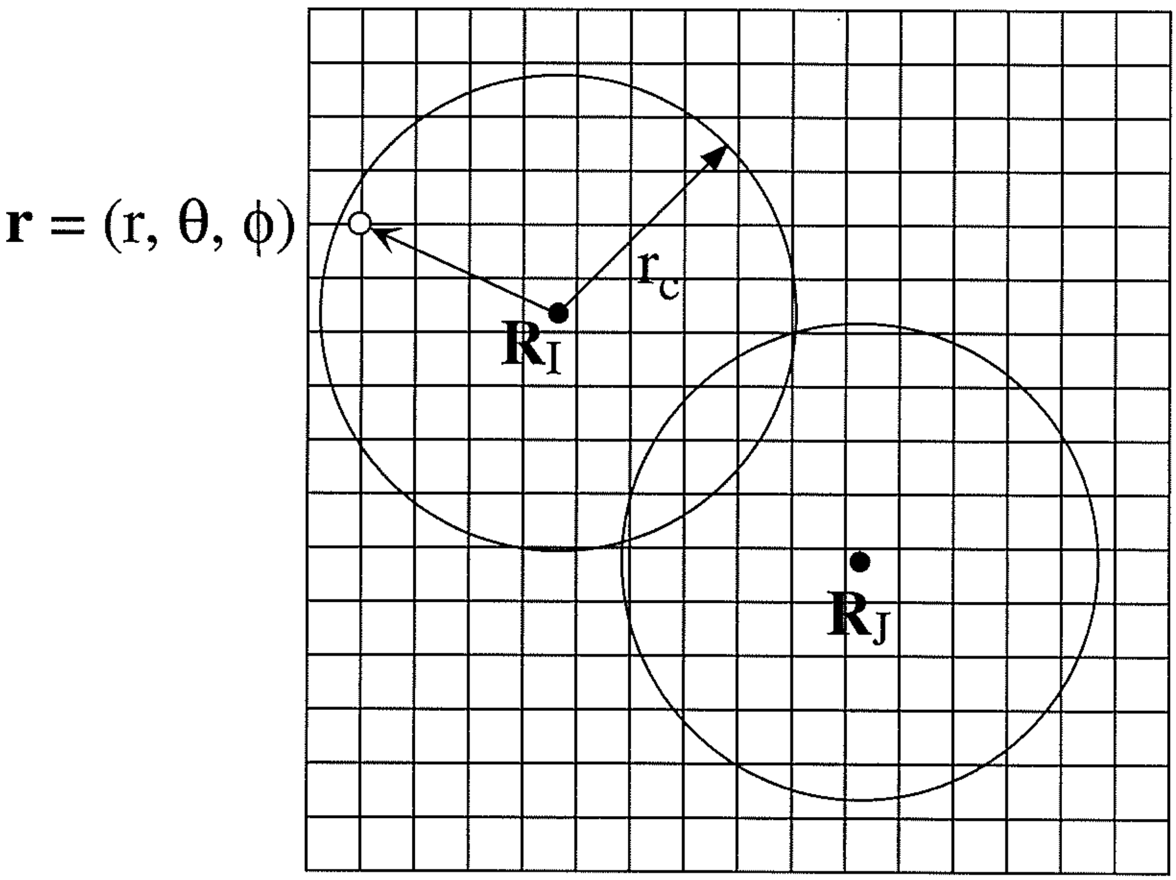
for each orbital n

$B_{lm}(n) \leftarrow \int d\mathbf{r}\, R_l^{PP}(r) \Delta V_l(r) Y_{lm}^*(\hat{r}) \psi_n(\mathbf{r}) \quad (l=0,\ldots,l_{max};\ m=-l,\ldots,l)$

$$\hat{V}_{NL}|\psi_n\rangle \mathrel{+}= \sum_{lm} \frac{B_{lm}(n)}{A_l} Y_{lm}(\hat{r}) \Delta V_l(r) R_l^{PP}(r)$$

The operation count $\propto N_I$ (# of ions) $\times$ N_B (# of bands)

$O(N_I N_B) = O(N^2)$!


r = (r, θ, φ)
r_c
R_I
R_J

Calculation of $B_{\ell m}(n)$

Using finite difference on a mesh with size Δ,

$$B^{I}_{\ell m}(n) = \Delta^3 \sum_{\{\mathbf{r} \,|\, |\mathbf{r}-\mathbf{R}_I| \in r_c\}} \underbrace{R^{PP}_{\ell}(|\mathbf{r}-\mathbf{R}_I|)\, \Delta V_{\ell}(|\mathbf{r}-\mathbf{R}_I|)}_{\text{interpolate tables}} Y^{*}_{\ell m}(\widehat{\mathbf{r}-\mathbf{R}_I})\, \psi_n(\mathbf{r}) \qquad (5)$$

where $\mathbf{r}$ are discrete mesh points.

Potential Problem of Eq. (5)

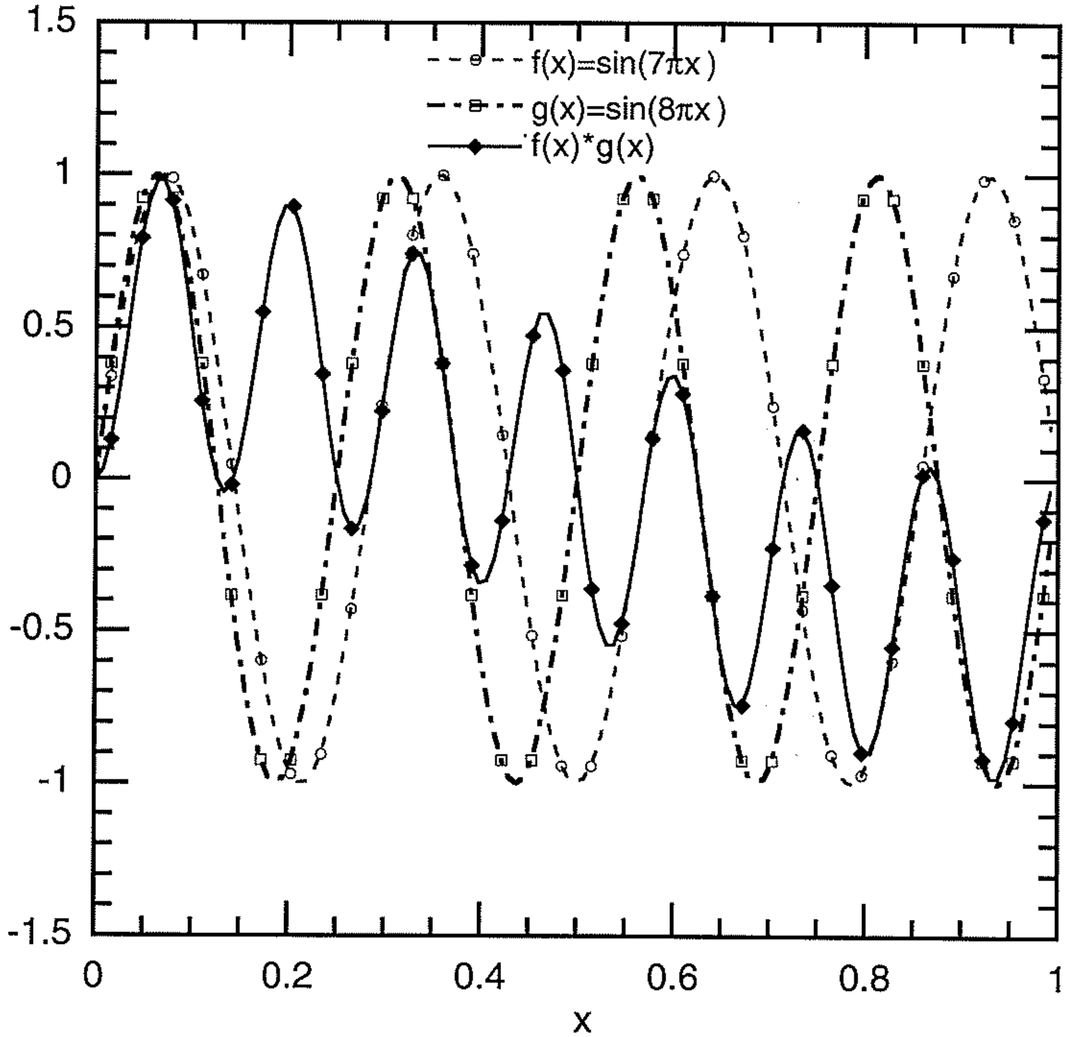
With mesh size Δ, the wave number to be represented is $-\pi/\Delta \le k \le \pi/\Delta$ for both $R^{PP}_{\ell}\Delta V_{\ell} Y^{*}_{\ell m}(\mathbf{r}-\mathbf{R}_I)$ and $\psi_n(\mathbf{r})$. If we multiply these two quantities, however, much larger periodicity can arise. For example,

$$\cos(kr)\cos(k'r) = \frac{1}{2}\left\{\cos[(k+k')r] + \cos[(k-k')r]\right\}$$

In principle, thus $k \sim 2\pi/\Delta$ component can result. The atomic pseudowavefunction can be highly oscillatory (i.e., high k component with a rough mesh can be quite large), and therefore the resulting wave cannot be represented on the same mesh.

Remedy (roughly stated)

Make high-k components of atomic pseudowavefunctions strictly zero so that the unrepresentable convolution will not arise.



f(x)=sin(7πx)
g(x)=sin(8πx)
f(x)*g(x)
1.5
1
0.5
0
-0.5
-1
-1.5
0
0.2
0.4
0.6
0.8
1
x