EAM と格子振動

by T.Koyama

１．中心場ポテンシャルとダイナミカルマトリックス

まず、歪んでいない結晶格子点の位置ベクトルを $\mathbf{R}$ とする。次に歪が生じた時の変位ベクトルを $\mathbf{u}(\mathbf{R})$ とすると、歪んだ後の原子の位置ベクトル $\mathbf{r}(\mathbf{R})$ は、

$$\mathbf{r}(\mathbf{R}) = \mathbf{R} + \mathbf{u}(\mathbf{R}) \tag{1}$$

にて与えられる。次に、原子間ポテンシャルを、$\phi(\mathbf{r})$ としよう。歪んでいない結晶の全内部エネルギーは、

$$U = \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'}\phi(\mathbf{R}-\mathbf{R}') = \frac{1}{2}N\sum_{\mathbf{R}\neq 0}\phi(\mathbf{R}) \tag{2}$$

にて計算される。N は全格子点数である。また同様に、歪んだ後の結晶の全内部エネルギーは、式(1)を用いて、

$$U = \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'}\phi\{\mathbf{r}(\mathbf{R})-\mathbf{r}(\mathbf{R}')\} = \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'}\phi\{\mathbf{R}-\mathbf{R}'+\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\} \tag{3}$$

にて与えられる。式(3)を３次元テイラー展開しよう。３次元テイラー展開の公式は、

$$\begin{aligned}
f(\mathbf{r}+\mathbf{a}) &= f(\mathbf{r}) + (\mathbf{a}\cdot\nabla)f(\mathbf{r}) + \frac{1}{2!}(\mathbf{a}\cdot\nabla)^2 f(\mathbf{r}) + \frac{1}{3!}(\mathbf{a}\cdot\nabla)^3 f(\mathbf{r}) + \cdots \\
&= f(x_1,x_2,x_3) + \left(a_1\frac{\partial}{\partial x_1} + a_2\frac{\partial}{\partial x_2} + a_3\frac{\partial}{\partial x_3}\right) f(x_1,x_2,x_3) \\
&\quad + \frac{1}{2!}\left(a_1\frac{\partial}{\partial x_1} + a_2\frac{\partial}{\partial x_2} + a_3\frac{\partial}{\partial x_3}\right)^2 f(x_1,x_2,x_3) + \frac{1}{3!}\left(a_1\frac{\partial}{\partial x_1} + a_2\frac{\partial}{\partial x_2} + a_3\frac{\partial}{\partial x_3}\right)^3 f(x_1,x_2,x_3) + \cdots \\
&= f(x_1,x_2,x_3) + \left(a_1\frac{\partial}{\partial x_1} + a_2\frac{\partial}{\partial x_2} + a_3\frac{\partial}{\partial x_3}\right) f(x_1,x_2,x_3) \\
&\quad + \frac{1}{2!}\left(a_1^2\frac{\partial^2}{\partial x_1^2} + a_2^2\frac{\partial^2}{\partial x_2^2} + a_3^2\frac{\partial^2}{\partial x_3^2} + 2a_1a_2\frac{\partial^2}{\partial x_1\partial x_2} + 2a_2a_3\frac{\partial^2}{\partial x_2\partial x_3} + 2a_3a_1\frac{\partial^2}{\partial x_3\partial x_1}\right) f(x_1,x_2,x_3) \\
&\quad + \cdots
\end{aligned}$$

である。これを用いて、式(3)を展開してみよう。

$$\begin{aligned}
U &= \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'}\phi\{\mathbf{R}-\mathbf{R}'+\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\} \\
&= \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'}\phi(\mathbf{R}-\mathbf{R}') + \frac{1}{2}\sum_{\mathbf{R}\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]\phi(\mathbf{R}-\mathbf{R}') \\
&\quad + \frac{1}{4}\sum_{\mathbf{R},\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]^2\phi(\mathbf{R}-\mathbf{R}') + \cdots
\end{aligned} \tag{4}$$

ここで、右辺第２項は、原子の平衡位置を与える式になるので、

$$\frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]\phi(\mathbf{R}-\mathbf{R}') = 0 \tag{5}$$

である。また第１項は、歪んでいない結晶の全内部エネルギーであるから、歪んだことによる過剰エネルギー分 E は、結局、第３項以降のみとなる。第４項以降を省略し、第３項のみを取り上げると、E は、

$$
\begin{aligned}
E &= \frac{1}{4}\sum_{\mathbf{R},\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]^2\phi(\mathbf{R}-\mathbf{R}') \\
&= \frac{1}{4}\sum_{\mathbf{R},\mathbf{R}',\mu,\nu=x,y,z}\{u_\mu(\mathbf{R})-u_\mu(\mathbf{R}')\}\frac{\partial^2\phi(\mathbf{R}-\mathbf{R}')}{\partial r_\mu \partial r_\nu}\{u_\nu(\mathbf{R})-u_\nu(\mathbf{R}')\} \\
&= \frac{1}{4}\sum_{\mathbf{R},\mathbf{R}',\mu,\nu=x,y,z}\{u_\mu(\mathbf{R})-u_\mu(\mathbf{R}')\}\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')\{u_\nu(\mathbf{R})-u_\nu(\mathbf{R}')\}
\end{aligned}
\tag{6}
$$

と表される。ここで、

$$
\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') \equiv \frac{\partial^2\phi(\mathbf{R}-\mathbf{R}')}{\partial r_\mu \partial r_\nu} \tag{7}
$$

と置いた。さらに

$$
D_{\mu\nu}(\mathbf{R}-\mathbf{R}') \equiv \delta_{\mathbf{R}\mathbf{R}'}\sum_{\mathbf{R}''}\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'')-\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') \tag{8}
$$

と置いて、式(6)を書き直すと、

$$
\begin{aligned}
E &= \frac{1}{4}\sum_{\mathbf{R},\mathbf{R}',\mu,\nu}\{u_\mu(\mathbf{R})-u_\mu(\mathbf{R}')\}\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')\{u_\nu(\mathbf{R})-u_\nu(\mathbf{R}')\} \\
&= \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}',\mu,\nu}u_\mu(\mathbf{R})D_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R}')
\end{aligned}
\tag{9}
$$

を得る。この変形は、

$$
\begin{aligned}
E &= \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}',\mu,\nu} u_\mu(\mathbf{R}) D_{\mu\nu}(\mathbf{R}-\mathbf{R}') u_\nu(\mathbf{R}') \\
&= \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}',\mu,\nu} u_\mu(\mathbf{R}) \left\{ \delta_{\mathbf{R}\mathbf{R}'} \sum_{\mathbf{R}''} \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'') - \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') \right\} u_\nu(\mathbf{R}') \\
&= \frac{1}{2}\sum_{\mathbf{R},\mu,\nu} \sum_{\mathbf{R}'} \left[u_\mu(\mathbf{R}) \left\{ \delta_{\mathbf{R}\mathbf{R}'} \sum_{\mathbf{R}''} \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'') \right\} u_\nu(\mathbf{R}') \right] - \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}',\mu,\nu} u_\mu(\mathbf{R}) \left\{ \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') \right\} u_\nu(\mathbf{R}') \\
&= \frac{1}{2}\sum_{\mathbf{R},\mu,\nu} \sum_{\mathbf{R}''} u_\mu(\mathbf{R}) \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'') u_\nu(\mathbf{R}) - \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}',\mu,\nu} u_\mu(\mathbf{R}) \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') u_\nu(\mathbf{R}') \\
&= \frac{1}{2}\sum_{\mathbf{R},\mu,\nu} \sum_{\mathbf{R}'} u_\mu(\mathbf{R}) \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') u_\nu(\mathbf{R}) - \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}',\mu,\nu} u_\mu(\mathbf{R}) \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') u_\nu(\mathbf{R}') \\
&= \frac{1}{4}\sum_{\mathbf{R},\mathbf{R}',\mu,\nu} \left[\begin{aligned} &u_\mu(\mathbf{R}) \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') u_\nu(\mathbf{R}) \\ &+ u_\mu(\mathbf{R}') \phi_{\mu\nu}(\mathbf{R}'-\mathbf{R}) u_\nu(\mathbf{R}') \end{aligned} \right] - \frac{1}{4}\sum_{\mathbf{R},\mathbf{R}',\mu,\nu} \left[\begin{aligned} &u_\mu(\mathbf{R}) \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') u_\nu(\mathbf{R}') \\ &+ u_\mu(\mathbf{R}') \phi_{\mu\nu}(\mathbf{R}'-\mathbf{R}) u_\nu(\mathbf{R}) \end{aligned} \right] \\
&= \frac{1}{4}\sum_{\mathbf{R},\mathbf{R}',\mu,\nu} \left[\begin{aligned} &u_\mu(\mathbf{R}) \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') u_\nu(\mathbf{R}) + u_\mu(\mathbf{R}') \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') u_\nu(\mathbf{R}') \\ &- u_\mu(\mathbf{R}) \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') u_\nu(\mathbf{R}') - u_\mu(\mathbf{R}') \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') u_\nu(\mathbf{R}) \end{aligned} \right] \\
&= \frac{1}{4}\sum_{\mathbf{R},\mathbf{R}',\mu,\nu} \{u_\mu(\mathbf{R}) - u_\mu(\mathbf{R}')\} \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') \{u_\nu(\mathbf{R}) - u_\nu(\mathbf{R}')\}
\end{aligned}
$$

より確認することが出来る。なおこの計算の際に、$\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') = \phi_{\mu\nu}(\mathbf{R}'-\mathbf{R})$ の関係を用いた。

さらに、一般的に、変位 $u_\mu(\mathbf{R}), u_\nu(\mathbf{R})$ と $D_{\mu\nu}(\mathbf{R}-\mathbf{R}')$ をベクトルおよびマトリックス表記すると、

$$
E = \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}',\mu,\nu} u_\mu(\mathbf{R}) D_{\mu\nu}(\mathbf{R}-\mathbf{R}') u_\nu(\mathbf{R}') = \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'} \mathbf{u}(\mathbf{R}) \mathbf{D}(\mathbf{R}-\mathbf{R}') \mathbf{u}(\mathbf{R}') \tag{10}
$$

となる。また $D_{\mu\nu}(\mathbf{R}-\mathbf{R}')$ に関する関係式として、

$$
\begin{aligned}
D_{\mu\nu}(\mathbf{R}-\mathbf{R}') &= D_{\mu\nu}(\mathbf{R}'-\mathbf{R}) \\
D_{\mu\nu}(\mathbf{R}-\mathbf{R}') &= D_{\nu\mu}(\mathbf{R}-\mathbf{R}')
\end{aligned} \tag{11-1}
$$

$$
\sum_{\mathbf{R}} D_{\mu\nu}(\mathbf{R}) = 0 \tag{11-2}
$$

が成立する。さてダイナミカルマトリックスは、

$$
\mathbf{D}(\mathbf{k}) = \sum_{\mathbf{R}} \mathbf{D}(\mathbf{R}) \exp(-i\mathbf{k}\cdot\mathbf{R}) \tag{12}
$$

と定義される。式(11-2)より、

$$\sum_{\mathbf{R}} D_{\mu\nu}(\mathbf{R}) = 0$$
$$D_{\mu\nu}(0) + \sum_{\mathbf{R},\mathbf{R}\neq 0} D_{\mu\nu}(\mathbf{R}) = 0 \tag{13}$$

であるので、これを用いて式(12)を変形すると、

$$\begin{aligned}
D_{\mu\nu}(\mathbf{k}) &= \sum_{\mathbf{R}} D_{\mu\nu}(\mathbf{R}) \exp(-i\mathbf{k}\cdot\mathbf{R}) \\
&= D_{\mu\nu}(0) + \sum_{\mathbf{R},\mathbf{R}\neq 0} D_{\mu\nu}(\mathbf{R}) \exp(-i\mathbf{k}\cdot\mathbf{R}) \\
&= -\sum_{\mathbf{R},\mathbf{R}\neq 0} D_{\mu\nu}(\mathbf{R}) + \sum_{\mathbf{R},\mathbf{R}\neq 0} D_{\mu\nu}(\mathbf{R}) \exp(-i\mathbf{k}\cdot\mathbf{R}) \\
&= -\sum_{\mathbf{R},\mathbf{R}\neq 0} D_{\mu\nu}(\mathbf{R}) \{1 - \exp(-i\mathbf{k}\cdot\mathbf{R})\} \\
&= -\sum_{\mathbf{R},\mathbf{R}\neq 0} \frac{1}{2}\left[D_{\mu\nu}(\mathbf{R})\{1 - \exp(-i\mathbf{k}\cdot\mathbf{R})\} + D_{\mu\nu}(-\mathbf{R})\{1 - \exp(i\mathbf{k}\cdot\mathbf{R})\}\right] \\
&= -\sum_{\mathbf{R},\mathbf{R}\neq 0} \frac{1}{2} D_{\mu\nu}(\mathbf{R})\left[2 - \{\exp(-i\mathbf{k}\cdot\mathbf{R}) + \exp(i\mathbf{k}\cdot\mathbf{R})\}\right] \\
&= -\sum_{\mathbf{R},\mathbf{R}\neq 0} D_{\mu\nu}(\mathbf{R})\left[1 - \cos(\mathbf{k}\cdot\mathbf{R})\right] \\
&= -2\sum_{\mathbf{R},\mathbf{R}\neq 0} D_{\mu\nu}(\mathbf{R}) \sin^2\left(\frac{1}{2}\mathbf{k}\cdot\mathbf{R}\right)
\end{aligned}$$

となる。特に、

$$\begin{aligned}
D_{\mu\nu}(\mathbf{k}) &= \sum_{\mathbf{R}} D_{\mu\nu}(\mathbf{R}) \exp(-i\mathbf{k}\cdot\mathbf{R}) \\
&= -\sum_{\mathbf{R},\mathbf{R}\neq 0} D_{\mu\nu}(\mathbf{R}) \{1 - \exp(-i\mathbf{k}\cdot\mathbf{R})\} \\
&= -\sum_{\mathbf{R},\mathbf{R}\neq 0} D_{\mu\nu}(\mathbf{R})\left[1 - \cos(\mathbf{k}\cdot\mathbf{R})\right] = -2\sum_{\mathbf{R},\mathbf{R}\neq 0} D_{\mu\nu}(\mathbf{R}) \sin^2\left(\frac{1}{2}\mathbf{k}\cdot\mathbf{R}\right)
\end{aligned} \tag{14}$$

の形式が実際の計算に使用される。

以上までの議論は、中心間力のみが作用するポテンシャルの場合であったが、次にポテンシャル表現として、EAM ポテンシャルを使用する場合について説明する。

2．EAM ポテンシャル場とダイナミカルマトリックス

まず歪んでいない結晶格子点の位置ベクトルを $\mathbf{R}$ とする。次に歪が生じた時の変位ベクトルを $\mathbf{u}(\mathbf{R})$ とすると、歪んだ後の原子の位置ベクトル $\mathbf{r}(\mathbf{R})$ は、

$$\mathbf{r}(\mathbf{R}) = \mathbf{R} + \mathbf{u}(\mathbf{R}) \tag{1}$$

にて与えられる。次に、EAM ポテンシャルに基づく、歪んでいない結晶の全内部エネルギーは、

$$U=\sum_{\mathbf{R}}F\left[\overline{\rho}(\mathbf{R})\right]+\frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'}\phi(\mathbf{R}-\mathbf{R}')=\sum_{\mathbf{R}}F\left[\sum_{\mathbf{R}'}\rho(\mathbf{R}-\mathbf{R}')\right]+\frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'}\phi(\mathbf{R}-\mathbf{R}') \tag{2}$$

$$\overline{\rho}(\mathbf{R})=\sum_{\mathbf{R}'(\mathbf{R}'\neq\mathbf{0})}\rho(\mathbf{R}-\mathbf{R}') \tag{3}$$

にて計算される。また、歪んだ後の結晶の全内部エネルギーは、式(1)を用いて、

$$\begin{aligned}U&=\sum_{\mathbf{R}}F\left[\sum_{\mathbf{R}'}\rho\{\mathbf{r}(\mathbf{R})-\mathbf{r}(\mathbf{R}')\}\right]+\frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'}\phi\{\mathbf{r}(\mathbf{R})-\mathbf{r}(\mathbf{R}')\}\\&=\sum_{\mathbf{R}}F\left[\sum_{\mathbf{R}'}\rho\{\mathbf{R}-\mathbf{R}'+\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\right]+\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\phi\{\mathbf{R}-\mathbf{R}'+\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\end{aligned} \tag{4}$$

にて与えられる。式(4)を３次元テイラー展開しよう。式(4)の第２項は、中心間距離のみに依存するポテンシャル場であるので、前章と同様にして、

$$\begin{aligned}&\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\phi\{\mathbf{R}-\mathbf{R}'+\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\\&\cong\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\phi(\mathbf{R}-\mathbf{R}')+\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla_{\mathbf{R}}]\phi(\mathbf{R}-\mathbf{R}')\\&\quad+\frac{1}{4}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla_{\mathbf{R}}]^2\phi(\mathbf{R}-\mathbf{R}')\\&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\phi(\mathbf{R}-\mathbf{R}')+\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}[u_\nu(\mathbf{R})-u_\nu(\mathbf{R}')]\frac{\partial\phi(\mathbf{R}-\mathbf{R}')}{\partial R_\nu}\\&\quad+\frac{1}{4}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}[u_\mu(\mathbf{R})-u_\mu(\mathbf{R}')]\frac{\partial^2\phi(\mathbf{R}-\mathbf{R}')}{\partial R_\mu\partial R_\nu}[u_\nu(\mathbf{R})-u_\nu(\mathbf{R}')]\\&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\phi(\mathbf{R}-\mathbf{R}')+\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}[u_\nu(\mathbf{R})-u_\nu(\mathbf{R}')]\phi_\nu(\mathbf{R}-\mathbf{R}')\\&\quad+\frac{1}{4}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}[u_\mu(\mathbf{R})-u_\mu(\mathbf{R}')]\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')[u_\nu(\mathbf{R})-u_\nu(\mathbf{R}')]\end{aligned} \tag{5}$$

と書き下すことが出来る。ここで、

$$
\begin{aligned}
&\frac{1}{4}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}[u_{\mu}(\mathbf{R})-u_{\mu}(\mathbf{R}')]\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')[u_{\nu}(\mathbf{R})-u_{\nu}(\mathbf{R}')] \\
&=\frac{1}{4}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_{\nu}(\mathbf{R})+\frac{1}{4}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R}')\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_{\nu}(\mathbf{R}') \\
&\quad-\frac{1}{4}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_{\nu}(\mathbf{R}')-\frac{1}{4}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R}')\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_{\nu}(\mathbf{R}) \\
&=\frac{1}{4}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_{\nu}(\mathbf{R})+\frac{1}{4}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\phi_{\mu\nu}(\mathbf{R}'-\mathbf{R})u_{\nu}(\mathbf{R}) \\
&\quad-\frac{1}{4}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_{\nu}(\mathbf{R}')-\frac{1}{4}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\phi_{\mu\nu}(\mathbf{R}'-\mathbf{R})u_{\nu}(\mathbf{R}') \\
&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_{\nu}(\mathbf{R})-\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_{\nu}(\mathbf{R}') \\
&=\frac{1}{2}\sum_{\mathbf{R}}u_{\mu}(\mathbf{R})\left[\sum_{\mathbf{R}'}\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')\right]\left[\sum_{\mathbf{R}''}\delta_{\mathbf{R}\mathbf{R}''}u_{\nu}(\mathbf{R}'')\right]-\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_{\nu}(\mathbf{R}') \\
&=\frac{1}{2}\sum_{\mathbf{R}}u_{\mu}(\mathbf{R})\left[\sum_{\mathbf{R}'}\sum_{\mathbf{R}''}\delta_{\mathbf{R}\mathbf{R}''}u_{\nu}(\mathbf{R}'')\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')\right]-\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_{\nu}(\mathbf{R}') \\
&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}''}u_{\mu}(\mathbf{R})\left\{\delta_{\mathbf{R}\mathbf{R}''}\sum_{\mathbf{R}'}\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')\right\}u_{\nu}(\mathbf{R}'')-\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_{\nu}(\mathbf{R}') \\
&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\left\{\delta_{\mathbf{R}\mathbf{R}'}\sum_{\mathbf{R}''}\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'')\right\}u_{\nu}(\mathbf{R}')-\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_{\nu}(\mathbf{R}') \\
&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\left\{\delta_{\mathbf{R}\mathbf{R}'}\sum_{\mathbf{R}''}\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'')-\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')\right\}u_{\nu}(\mathbf{R}')
\end{aligned}
\tag{6}
$$

であるので、式(5)は最終的に

$$
\begin{aligned}
&\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\phi\{\mathbf{R}-\mathbf{R}'+\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\} \\
&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\phi(\mathbf{R}-\mathbf{R}')+\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}[u_{\nu}(\mathbf{R})-u_{\nu}(\mathbf{R}')]\phi_{\nu}(\mathbf{R}-\mathbf{R}') \\
&\quad+\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_{\mu}(\mathbf{R})\left\{\delta_{\mathbf{R}\mathbf{R}'}\sum_{\mathbf{R}''}\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'')-\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')\right\}u_{\nu}(\mathbf{R}')
\end{aligned}
\tag{7}
$$

と変形できる。右辺第１項は、変位がない場合に対応し、第２項は、全エネルギーの１階微分項にふくまれるため、最終的には消える項である。

さて、次に式(4)の右辺第１項を書き下そう。この場合、位置および変位場に関する関数が陰関数となっており、さらに積分変数(和変数)の範囲が、複雑であるので、以下、順に整理して説明する。まず変位場が 0 である時の埋込関数 F は、

$$
F\{\bar{\rho}(\mathbf{R})\}=F\left[\sum_{\mathbf{R}'}\rho(\mathbf{R}-\mathbf{R}')\right]
$$

である。まず $\mathbf{R}$ に対して $\mathbf{u}(\mathbf{R})$ だけ変位が発生した場合、$\bar{\rho}(\mathbf{R}+\mathbf{u}(\mathbf{R}))$ は次のように展開で

きる。

$$\overline{\rho}(\mathbf{R}+\mathbf{u}(\mathbf{R}))=\overline{\rho}(\mathbf{R})+[\mathbf{u}(\mathbf{R})\cdot\nabla]\overline{\rho}(\mathbf{R})+\frac{1}{2}[\mathbf{u}(\mathbf{R})\cdot\nabla]^2\overline{\rho}(\mathbf{R}) \tag{8}$$

また $\overline{\rho}(\mathbf{R}+\mathbf{u}(\mathbf{R}))$ 自身はもともと、 $\overline{\rho}(\mathbf{R}+\mathbf{u}(\mathbf{R}))=\sum_{\mathbf{R}'}\rho\{\mathbf{R}-\mathbf{R}'+\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}$ であるので、$\rho\{\mathbf{R}-\mathbf{R}'+\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}$ を $\mathbf{u}(\mathbf{R}')$ について展開すると、

$$\begin{aligned}\overline{\rho}(\mathbf{R}+\mathbf{u}(\mathbf{R}))&=\sum_{\mathbf{R}'}\rho\{\mathbf{R}+\mathbf{u}(\mathbf{R})-\mathbf{R}'-\mathbf{u}(\mathbf{R}')\}\\&=\sum_{\mathbf{R}'}\rho\{\mathbf{R}+\mathbf{u}(\mathbf{R})-\mathbf{R}'\}+\sum_{\mathbf{R}'}[\{-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]\rho\{\mathbf{R}+\mathbf{u}(\mathbf{R})-\mathbf{R}'\}\\&\quad+\frac{1}{2}\sum_{\mathbf{R}'}[\{-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]^2\rho\{\mathbf{R}+\mathbf{u}(\mathbf{R})-\mathbf{R}'\}\end{aligned} \tag{9}$$

となる。ここで、積分(サンメーション)は $\mathbf{R}'$ について取られているので、この積分の内部の変数は $\mathbf{R}'$ と $\mathbf{u}(\mathbf{R}')$ である。したがって、展開は $\mathbf{u}(\mathbf{R}')$ のみについて行わなくてはならない。式(8)の $\overline{\rho}(\mathbf{R})$ は、式(9)において $\mathbf{u}(\mathbf{R})=0$ にした場合に他ならないので、式(9)に $\mathbf{u}(\mathbf{R})=0$ を代入して、

$$\begin{aligned}\overline{\rho}(\mathbf{R})&=\sum_{\mathbf{R}'}\rho\{\mathbf{R}-\mathbf{R}'-\mathbf{u}(\mathbf{R}')\}\\&=\sum_{\mathbf{R}'}\rho\{\mathbf{R}-\mathbf{R}'\}+\sum_{\mathbf{R}'}[\{-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]\rho\{\mathbf{R}-\mathbf{R}'\}+\frac{1}{2}\sum_{\mathbf{R}'}[\{-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]^2\rho\{\mathbf{R}-\mathbf{R}'\}\end{aligned}$$

となる。これを式(8)に代入する。

$$
\begin{aligned}
&\bar{\rho}(\mathbf{R}+\mathbf{u}(\mathbf{R})) \\
&= \bar{\rho}(\mathbf{R}) + [\mathbf{u}(\mathbf{R})\cdot\nabla]\bar{\rho}(\mathbf{R}) + \frac{1}{2}[\mathbf{u}(\mathbf{R})\cdot\nabla]^2\bar{\rho}(\mathbf{R}) \\
&= \sum_{\mathbf{R}'}\rho\{\mathbf{R}-\mathbf{R}'\} + \sum_{\mathbf{R}'}[\{-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]\rho\{\mathbf{R}-\mathbf{R}'\} + \frac{1}{2}\sum_{\mathbf{R}'}[\{-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]^2\rho\{\mathbf{R}-\mathbf{R}'\} \\
&+[\mathbf{u}(\mathbf{R})\cdot\nabla]\left\{\sum_{\mathbf{R}'}\rho\{\mathbf{R}-\mathbf{R}'\} + \sum_{\mathbf{R}'}[\{-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]\rho\{\mathbf{R}-\mathbf{R}'\} + \frac{1}{2}\sum_{\mathbf{R}'}[\{-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]^2\rho\{\mathbf{R}-\mathbf{R}'\}\right\} \\
&+\frac{1}{2}[\mathbf{u}(\mathbf{R})\cdot\nabla]^2\left\{\sum_{\mathbf{R}'}\rho\{\mathbf{R}-\mathbf{R}'\} + \sum_{\mathbf{R}'}[\{-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]\rho\{\mathbf{R}-\mathbf{R}'\} + \frac{1}{2}\sum_{\mathbf{R}'}[\{-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]^2\rho\{\mathbf{R}-\mathbf{R}'\}\right\} \\
&\cong \sum_{\mathbf{R}'}\rho(\mathbf{R}-\mathbf{R}') + \sum_{\mathbf{R}'}[\{-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]\rho(\mathbf{R}-\mathbf{R}') + [\mathbf{u}(\mathbf{R})\cdot\nabla]\sum_{\mathbf{R}'}\rho(\mathbf{R}-\mathbf{R}') \\
&\quad + \frac{1}{2}\sum_{\mathbf{R}'}[\{-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]^2\rho(\mathbf{R}-\mathbf{R}') + \frac{1}{2}[\mathbf{u}(\mathbf{R})\cdot\nabla]^2\sum_{\mathbf{R}'}\rho(\mathbf{R}-\mathbf{R}') \\
&\quad + [\mathbf{u}(\mathbf{R})\cdot\nabla]\sum_{\mathbf{R}'}[\{-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]\rho(\mathbf{R}-\mathbf{R}') \\
&= \sum_{\mathbf{R}'}\rho(\mathbf{R}-\mathbf{R}') + [\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]\sum_{\mathbf{R}'}\rho(\mathbf{R}-\mathbf{R}') \\
&\quad + \frac{1}{2}\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]^2\rho(\mathbf{R}-\mathbf{R}')
\end{aligned}
$$

したがって、埋込関数は、

$$
\begin{aligned}
&\sum_{\mathbf{R}} F\left\{\sum_{\mathbf{R}'}\rho\{\mathbf{R}-\mathbf{R}'+\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\right\} \\
&= \sum_{\mathbf{R}} F\left\{\begin{aligned}&\sum_{\mathbf{R}'}\rho(\mathbf{R}-\mathbf{R}') + \sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]\rho(\mathbf{R}-\mathbf{R}') \\ &+\frac{1}{2}\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]^2\rho(\mathbf{R}-\mathbf{R}')\end{aligned}\right\} \\
&= \sum_{\mathbf{R}} F\left[\bar{\rho}(\mathbf{R}) + \Delta\bar{\rho}(\mathbf{R})\right]
\end{aligned}
\tag{10}
$$

$$
\Delta\bar{\rho}(\mathbf{R}) = \sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]\rho(\mathbf{R}-\mathbf{R}') + \frac{1}{2}\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla]^2\rho(\mathbf{R}-\mathbf{R}') \tag{11}
$$

と展開された。さらに今後は、F を $\bar{\rho}$ にて展開し、変位場に関する 2 次の項まで取ると、式(10)は、式(11)を用いて、

$$
\begin{aligned}
&\sum_{\mathbf{R}} F\left[\bar{\rho}(\mathbf{R})+\Delta\bar{\rho}(\mathbf{R})\right] \\
&= \sum_{\mathbf{R}} F\left[\bar{\rho}(\mathbf{R})\right] + \sum_{\mathbf{R}}\left[\Delta\bar{\rho}(\mathbf{R})\cdot\nabla_{\bar{\rho}}\right]F\left[\bar{\rho}(\mathbf{R})\right] + \frac{1}{2}\sum_{\mathbf{R}}\left[\Delta\bar{\rho}(\mathbf{R})\cdot\nabla_{\bar{\rho}}\right]^2 F\left[\bar{\rho}(\mathbf{R})\right] \\
&= \sum_{\mathbf{R}} F\left[\bar{\rho}(\mathbf{R})\right] + \sum_{\mathbf{R}}\left\{\left(\begin{array}{l}\displaystyle\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla_{\mathbf{R}}]\rho(\mathbf{R}-\mathbf{R}') \\ \displaystyle+\frac{1}{2}\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla_{\mathbf{R}}]^2\rho(\mathbf{R}-\mathbf{R}')\end{array}\right)\cdot\nabla_{\bar{\rho}}\right\}F\left[\bar{\rho}(\mathbf{R})\right] \\
&\quad+\frac{1}{2}\sum_{\mathbf{R}}\left\{\left(\begin{array}{l}\displaystyle\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla_{\mathbf{R}}]\rho(\mathbf{R}-\mathbf{R}') \\ \displaystyle+\frac{1}{2}\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla_{\mathbf{R}}]^2\rho(\mathbf{R}-\mathbf{R}')\end{array}\right)\cdot\nabla_{\bar{\rho}}\right\}^2 F\left[\bar{\rho}(\mathbf{R})\right] \\
&\cong \sum_{\mathbf{R}} F\left[\bar{\rho}(\mathbf{R})\right] + \sum_{\mathbf{R}}\left\{\left(\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla_{\mathbf{R}}]\rho(\mathbf{R}-\mathbf{R}')\right)\cdot\nabla_{\bar{\rho}}\right\}F\left[\bar{\rho}(\mathbf{R})\right] \\
&\quad+\frac{1}{2}\sum_{\mathbf{R}}\left\{\left(\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla_{\mathbf{R}}]^2\rho(\mathbf{R}-\mathbf{R}')\right)\cdot\nabla_{\bar{\rho}}\right\}F\left[\bar{\rho}(\mathbf{R})\right] \\
&\quad+\frac{1}{2}\sum_{\mathbf{R}}\left\{\left(\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla_{\mathbf{R}}]\rho(\mathbf{R}-\mathbf{R}')\right)\cdot\nabla_{\bar{\rho}}\right\}^2 F\left[\bar{\rho}(\mathbf{R})\right] \qquad (12)
\end{aligned}
$$

となる。ここで、位置 $\mathbf{R}$ と $\bar{\rho}$ に関する微分が区別できるように、$\nabla_{\mathbf{R}},\nabla_{\bar{\rho}}$ とした。式(12)の最後の２項は、

$$
\begin{aligned}
&\frac{1}{2}\sum_{\mathbf{R}}\left\{\left(\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla_{\mathbf{R}}]^2\rho(\mathbf{R}-\mathbf{R}')\right)\cdot\nabla_{\bar{\rho}}\right\}F\left[\bar{\rho}(\mathbf{R})\right] \\
&=\frac{1}{2}\sum_{\mathbf{R}}\left\{\sum_{\mathbf{R}'}[u_\mu(\mathbf{R})-u_\mu(\mathbf{R}')]\frac{\partial^2\rho(\mathbf{R}-\mathbf{R}')}{\partial R_\mu\partial R_\nu}[u_\nu(\mathbf{R})-u_\nu(\mathbf{R}')]\right\}\left(\frac{\partial F}{\partial\bar{\rho}}\right) \qquad (13) \\
&=\frac{1}{2}F'(\bar{\rho})\sum_{\mathbf{R}}\sum_{\mathbf{R}'}[u_\mu(\mathbf{R})-u_\mu(\mathbf{R}')]\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')[u_\nu(\mathbf{R})-u_\nu(\mathbf{R}')]
\end{aligned}
$$

$$
\begin{aligned}
&\frac{1}{2}\sum_{\mathbf{R}}\left\{\left(\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla_{\mathbf{R}}]\rho(\mathbf{R}-\mathbf{R}')\right)\cdot\nabla_{\bar{\rho}}\right\}^2 F\left[\bar{\rho}(\mathbf{R})\right] \\
&=\frac{1}{2}\sum_{\mathbf{R}}\left\{\sum_{\mathbf{R}'}\{u_\mu(\mathbf{R})-u_\mu(\mathbf{R}')\}\frac{\partial\rho(\mathbf{R}-\mathbf{R}')}{\partial R_\mu}\right)\left(\frac{\partial^2 F}{\partial\bar{\rho}^2}\right)\left(\sum_{\mathbf{R}'}\{u_\nu(\mathbf{R})-u_\nu(\mathbf{R}')\}\frac{\partial\rho(\mathbf{R}-\mathbf{R}')}{\partial R_\nu}\right\} \qquad (14) \\
&=\frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\{u_\mu(\mathbf{R})-u_\mu(\mathbf{R}')\}\rho_\mu(\mathbf{R}-\mathbf{R}')\sum_{\mathbf{R}''}\{u_\nu(\mathbf{R})-u_\nu(\mathbf{R}'')\}\rho_\nu(\mathbf{R}-\mathbf{R}'')
\end{aligned}
$$

と変形される。したがって、埋込関数は、

$$
\begin{aligned}
&\sum_{\mathbf{R}} F\left[\bar{\rho}(\mathbf{R})+\Delta\bar{\rho}(\mathbf{R})\right] \\
&=\sum_{\mathbf{R}} F\left[\bar{\rho}(\mathbf{R})\right]+\sum_{\mathbf{R}}\left[\left\{\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla_{\mathbf{R}}]\rho(\mathbf{R}-\mathbf{R}')\right\}\cdot\nabla_{\bar{\rho}}\right]F\left[\bar{\rho}(\mathbf{R})\right] \\
&\quad+\frac{1}{2}F'(\bar{\rho})\sum_{\mathbf{R}}\sum_{\mathbf{R}'}[u_\mu(\mathbf{R})-u_\mu(\mathbf{R}')]\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')[u_\nu(\mathbf{R})-u_\nu(\mathbf{R}')] \\
&\quad+\frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\{u_\mu(\mathbf{R})-u_\mu(\mathbf{R}')\}\rho_\mu(\mathbf{R}-\mathbf{R}')\sum_{\mathbf{R}''}\{u_\nu(\mathbf{R})-u_\nu(\mathbf{R}'')\}\rho_\nu(\mathbf{R}-\mathbf{R}'')
\end{aligned}
\tag{15}
$$

となる。第３項と第４項をもう少し書き下そう。

$$
\begin{aligned}
&\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}[u_\mu(\mathbf{R})-u_\mu(\mathbf{R}')]\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')[u_\nu(\mathbf{R})-u_\nu(\mathbf{R}')] \\
&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\left\{\begin{array}{l}u_\mu(\mathbf{R})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R})+u_\mu(\mathbf{R}')\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R}') \\ -u_\mu(\mathbf{R})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R}')-u_\mu(\mathbf{R}')\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R})\end{array}\right\} \\
&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_\mu(\mathbf{R})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R})+\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_\mu(\mathbf{R}')\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R}') \\
&\quad-\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_\mu(\mathbf{R})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R}')-\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_\mu(\mathbf{R}')\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R}) \\
&=\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_\mu(\mathbf{R})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R})-\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_\mu(\mathbf{R})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R}') \\
&=\sum_{\mathbf{R}}u_\mu(\mathbf{R})\left[\left\{\sum_{\mathbf{R}'}\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')\right\}\left\{\sum_{\mathbf{R}''}\delta_{\mathbf{R}\mathbf{R}''}u_\nu(\mathbf{R}'')\right\}\right]-\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_\mu(\mathbf{R})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R}') \\
&=\sum_{\mathbf{R}}u_\mu(\mathbf{R})\sum_{\mathbf{R}''}u_\nu(\mathbf{R}'')\left\{\delta_{\mathbf{R}\mathbf{R}''}\sum_{\mathbf{R}'}\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')\right\}-\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_\mu(\mathbf{R})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R}') \\
&=\sum_{\mathbf{R}}u_\mu(\mathbf{R})\sum_{\mathbf{R}'}u_\nu(\mathbf{R}')\left\{\delta_{\mathbf{R}\mathbf{R}'}\sum_{\mathbf{R}''}\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}'')\right\}-\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_\mu(\mathbf{R})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R}') \\
&=\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_\mu(\mathbf{R})\left\{\delta_{\mathbf{R}\mathbf{R}'}\sum_{\mathbf{R}''}\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}'')-\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')\right\}u_\nu(\mathbf{R}')
\end{aligned}
$$

および

$$
\begin{aligned}
&\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\{u_\mu(\mathbf{R})-u_\mu(\mathbf{R}')\}\rho_\mu(\mathbf{R}-\mathbf{R}')\sum_{\mathbf{R}''}\{u_\nu(\mathbf{R})-u_\nu(\mathbf{R}'')\}\rho_\nu(\mathbf{R}-\mathbf{R}'') \\
&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\sum_{\mathbf{R}''}[u_\mu(\mathbf{R})-u_\mu(\mathbf{R}')]\rho_\mu(\mathbf{R}-\mathbf{R}')\rho_\nu(\mathbf{R}-\mathbf{R}'')[u_\nu(\mathbf{R})-u_\nu(\mathbf{R}'')] \\
&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\sum_{\mathbf{R}''}\left\{\begin{aligned}&u_\mu(\mathbf{R})\rho_\mu(\mathbf{R}-\mathbf{R}')\rho_\nu(\mathbf{R}-\mathbf{R}'')u_\nu(\mathbf{R})+u_\mu(\mathbf{R}')\rho_\mu(\mathbf{R}-\mathbf{R}')\rho_\nu(\mathbf{R}-\mathbf{R}'')u_\nu(\mathbf{R}'')\\ &-u_\mu(\mathbf{R})\rho_\mu(\mathbf{R}-\mathbf{R}')\rho_\nu(\mathbf{R}-\mathbf{R}'')u_\nu(\mathbf{R}'')-u_\mu(\mathbf{R}')\rho_\mu(\mathbf{R}-\mathbf{R}')\rho_\nu(\mathbf{R}-\mathbf{R}'')u_\nu(\mathbf{R})\end{aligned}\right\} \\
&=\frac{1}{2}\sum_{\mathbf{R}}u_\mu(\mathbf{R})u_\nu(\mathbf{R})\sum_{\mathbf{R}'}\rho_\mu(\mathbf{R}-\mathbf{R}')\sum_{\mathbf{R}''}\rho_\nu(\mathbf{R}-\mathbf{R}'') \\
&\quad+\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_\mu(\mathbf{R}')\rho_\mu(\mathbf{R}-\mathbf{R}')\sum_{\mathbf{R}''}\rho_\nu(\mathbf{R}-\mathbf{R}'')u_\nu(\mathbf{R}'') \\
&\quad-\frac{1}{2}\sum_{\mathbf{R}}u_\mu(\mathbf{R})\sum_{\mathbf{R}'}\rho_\mu(\mathbf{R}-\mathbf{R}')\sum_{\mathbf{R}''}\rho_\nu(\mathbf{R}-\mathbf{R}'')u_\nu(\mathbf{R}'') \\
&\quad-\frac{1}{2}\sum_{\mathbf{R}}u_\nu(\mathbf{R})\sum_{\mathbf{R}'}u_\mu(\mathbf{R}')\rho_\mu(\mathbf{R}-\mathbf{R}')\sum_{\mathbf{R}''}\rho_\nu(\mathbf{R}-\mathbf{R}'') \\
&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_\mu(\mathbf{R}')\rho_\mu(\mathbf{R}-\mathbf{R}')\sum_{\mathbf{R}''}\rho_\nu(\mathbf{R}-\mathbf{R}'')u_\nu(\mathbf{R}'')
\end{aligned}
$$

となる。ここで$\sum_{\mathbf{R}'}\rho_\mu(\mathbf{R}-\mathbf{R}')=0$の関係(電荷勾配の総和は０)を用いた。これより、式(15)は

$$
\begin{aligned}
&\sum_{\mathbf{R}}F\left[\bar{\rho}(\mathbf{R})+\Delta\bar{\rho}(\mathbf{R})\right] \\
&=\sum_{\mathbf{R}}F\left[\bar{\rho}(\mathbf{R})\right]+\sum_{\mathbf{R}}\left\{\sum_{\mathbf{R}'}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R}')\}\cdot\nabla_{\mathbf{R}}]\rho(\mathbf{R}-\mathbf{R}')\right\}\cdot\nabla_{\bar{\rho}}\left\{F\left[\bar{\rho}(\mathbf{R})\right]\right. \\
&\quad+F'(\bar{\rho})\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_\mu(\mathbf{R})\left\{\delta_{\mathbf{R}\mathbf{R}'}\sum_{\mathbf{R}''}\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}'')-\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')\right\}u_\nu(\mathbf{R}') \\
&\quad+\frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{R}}\sum_{\mathbf{R}'}u_\mu(\mathbf{R}')\rho_\mu(\mathbf{R}-\mathbf{R}')\sum_{\mathbf{R}''}\rho_\nu(\mathbf{R}-\mathbf{R}'')u_\nu(\mathbf{R}'')
\end{aligned}
\tag{16}
$$

と表現される。右辺第１項は変位がない場合に対応し、第２項は全エネルギーの１階微分項に含まれるので、最終的には消える項である。

以上より、式(7)と(16)から変位場に依存する過剰エネルギーE_Dのみを取り出すと、

$$
\begin{aligned}
E_D &= \frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'} u_\mu(\mathbf{R})\left\{\delta_{\mathbf{RR}'}\sum_{\mathbf{R}''}\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'')-\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')\right\}u_\nu(\mathbf{R}') \\
&\quad + F'(\bar{\rho})\sum_{\mathbf{R}}\sum_{\mathbf{R}'} u_\mu(\mathbf{R})\left\{\delta_{\mathbf{RR}'}\sum_{\mathbf{R}''}\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}'')-\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')\right\}u_\nu(\mathbf{R}') \\
&\quad + \frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{R}}\sum_{\mathbf{R}'} u_\mu(\mathbf{R}')\rho_\mu(\mathbf{R}-\mathbf{R}')\sum_{\mathbf{R}''}\rho_\nu(\mathbf{R}-\mathbf{R}'')u_\nu(\mathbf{R}'') \\
&= \frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'} u_\mu(\mathbf{R})\left\{\begin{aligned}&\delta_{\mathbf{RR}'}\sum_{\mathbf{R}''}\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'')-\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') \\ &+2F'(\bar{\rho})\delta_{\mathbf{RR}'}\sum_{\mathbf{R}''}\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}'')-2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')\end{aligned}\right\}u_\nu(\mathbf{R}') \\
&\quad + \frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{R}}\sum_{\mathbf{R}'} u_\mu(\mathbf{R}')\rho_\mu(\mathbf{R}-\mathbf{R}')\sum_{\mathbf{R}''}\rho_\nu(\mathbf{R}-\mathbf{R}'')u_\nu(\mathbf{R}'') \\
&= \frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'} u_\mu(\mathbf{R})\left\{\begin{aligned}&\delta_{\mathbf{RR}'}\left[2F'(\bar{\rho})\sum_{\mathbf{R}''}\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}'')+\sum_{\mathbf{R}''}\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'')\right] \\ &-2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')-\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')\end{aligned}\right\}u_\nu(\mathbf{R}') \\
&\quad + \frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{R}}\left\{\sum_{\mathbf{R}'} u_\mu(\mathbf{R}')\rho_\mu(\mathbf{R}-\mathbf{R}')\right\}\left\{\sum_{\mathbf{R}''}\rho_\nu(\mathbf{R}-\mathbf{R}'')u_\nu(\mathbf{R}'')\right\} \\
&= \frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'} u_\mu(\mathbf{R})\left\{\begin{aligned}&\delta_{\mathbf{RR}'}\sum_{\mathbf{R}''}\left[2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}'')+\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'')\right] \\ &-2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}')-\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}')\end{aligned}\right\}u_\nu(\mathbf{R}') \\
&\quad + \frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{R}}\left\{\sum_{\mathbf{R}'} u_\mu(\mathbf{R}')\rho_\mu(\mathbf{R}-\mathbf{R}')\right\}\left\{\sum_{\mathbf{R}''}\rho_\nu(\mathbf{R}-\mathbf{R}'')u_\nu(\mathbf{R}'')\right\}
\end{aligned} \tag{17}
$$

を得る。なお、ここで、

$$
\begin{aligned}
\phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') &\equiv \frac{\partial^2\phi(\mathbf{R}-\mathbf{R}')}{\partial r_\mu \partial r_\nu} \\
\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}') &\equiv \frac{\partial^2\rho(\mathbf{R}-\mathbf{R}')}{\partial r_\mu \partial r_\nu} \\
\rho_\mu(\mathbf{R}-\mathbf{R}') &\equiv \frac{\partial\rho(\mathbf{R}-\mathbf{R}')}{\partial r_\mu}
\end{aligned} \tag{18}
$$

である。ちなみに、式(7)と(16)から座標に関する１階微分項を取り出すと、

$$
\begin{aligned}
&\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R'}}[u_\nu(\mathbf{R})-u_\nu(\mathbf{R'})]\phi_\nu(\mathbf{R}-\mathbf{R'})+\sum_{\mathbf{R}}\left\{\sum_{\mathbf{R'}}[\{\mathbf{u}(\mathbf{R})-\mathbf{u}(\mathbf{R'})\}\cdot\nabla_{\mathbf{R}}]\rho(\mathbf{R}-\mathbf{R'})\right\}\nabla_{\bar{\rho}}F\left[\bar{\rho}(\mathbf{R})\right]\\
&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R'}}[u_\nu(\mathbf{R})-u_\nu(\mathbf{R'})]\phi_\nu(\mathbf{R}-\mathbf{R'})+\sum_{\mathbf{R}}\left\{\sum_{\mathbf{R'}}[u_\nu(\mathbf{R})-u_\nu(\mathbf{R'})]\rho_\nu(\mathbf{R}-\mathbf{R'})\right\}F'\\
&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R'}}[u_\nu(\mathbf{R})-u_\nu(\mathbf{R'})]\phi_\nu(\mathbf{R}-\mathbf{R'})+\sum_{\mathbf{R}}\sum_{\mathbf{R'}}F'[u_\nu(\mathbf{R})-u_\nu(\mathbf{R'})]\rho_\nu(\mathbf{R}-\mathbf{R'})\\
&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R'}}\left[2F'\rho_\nu(\mathbf{R}-\mathbf{R'})+\phi_\nu(\mathbf{R}-\mathbf{R'})\right][u_\nu(\mathbf{R})-u_\nu(\mathbf{R'})]\\
&=\frac{1}{2}\sum_{\mathbf{R}}u_\nu(\mathbf{R})\left\{2F'\sum_{\mathbf{R'}}\rho_\nu(\mathbf{R}-\mathbf{R'})+\sum_{\mathbf{R'}}\phi_\nu(\mathbf{R}-\mathbf{R'})\right\}-\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R'}}\left[2F'\rho_\nu(\mathbf{R}-\mathbf{R'})+\phi_\nu(\mathbf{R}-\mathbf{R'})\right]u_\nu(\mathbf{R'})\\
&=-\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R'}}\left[2F'\rho_\nu(\mathbf{R}-\mathbf{R'})+\phi_\nu(\mathbf{R}-\mathbf{R'})\right]u_\nu(\mathbf{R'})=0\\
&\therefore\ \sum_{\mathbf{R}}\sum_{\mathbf{R'}}\left[2F'\rho_\nu(\mathbf{R}-\mathbf{R'})+\phi_\nu(\mathbf{R}-\mathbf{R'})\right]u_\nu(\mathbf{R'})=0
\end{aligned}
\tag{19}
$$

の関係式を得る。

さて、式(17)において、

$$
\begin{aligned}
A_{\mu\nu}(\mathbf{R}-\mathbf{R'})\equiv{}&\delta_{\mathbf{RR'}}\sum_{\mathbf{R''}}\left[2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R''})+\phi_{\mu\nu}(\mathbf{R}-\mathbf{R''})\right]\\
&-2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R'})-\phi_{\mu\nu}(\mathbf{R}-\mathbf{R'})
\end{aligned}
\tag{20}
$$

と置いて、式(17)を書き直すと、

$$
\begin{aligned}
E_D={}&\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R'}}u_\mu(\mathbf{R})\left\{\begin{aligned}&\delta_{\mathbf{RR'}}\sum_{\mathbf{R''}}\left[2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R''})+\phi_{\mu\nu}(\mathbf{R}-\mathbf{R''})\right]\\&-2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R'})-\phi_{\mu\nu}(\mathbf{R}-\mathbf{R'})\end{aligned}\right\}u_\nu(\mathbf{R'})\\
&+\frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{R}}\left\{\sum_{\mathbf{R'}}u_\mu(\mathbf{R'})\rho_\mu(\mathbf{R}-\mathbf{R'})\right\}\left\{\sum_{\mathbf{R''}}\rho_\nu(\mathbf{R}-\mathbf{R''})u_\nu(\mathbf{R''})\right\}\\
={}&\frac{1}{2}\sum_{\mathbf{R},\mathbf{R'}}u_\mu(\mathbf{R})A_{\mu\nu}(\mathbf{R}-\mathbf{R'})u_\nu(\mathbf{R'})\\
&+\frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{R}}\left\{\sum_{\mathbf{R'}}u_\mu(\mathbf{R'})\rho_\mu(\mathbf{R}-\mathbf{R'})\right\}\left\{\sum_{\mathbf{R''}}\rho_\nu(\mathbf{R}-\mathbf{R''})u_\nu(\mathbf{R''})\right\}
\end{aligned}
\tag{21}
$$

を得る。さらに一般的に、変位$u_\mu(\mathbf{R}),\,u_\nu(\mathbf{R})\,,A_{\mu\nu}(\mathbf{R}-\mathbf{R'})$をベクトルおよびマトリックス表記すると、

$$
\begin{aligned}
E_D &= \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'} u_\mu(\mathbf{R}) A_{\mu\nu}(\mathbf{R}-\mathbf{R}') u_\nu(\mathbf{R}') \\
&\quad + \frac{1}{2} F''(\bar{\rho}) \sum_{\mathbf{R}} \left\{ \sum_{\mathbf{R}'} u_\mu(\mathbf{R}') \rho_\mu(\mathbf{R}-\mathbf{R}') \right\} \left\{ \sum_{\mathbf{R}''} \rho_\nu(\mathbf{R}-\mathbf{R}'') u_\nu(\mathbf{R}'') \right\} \\
&= \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'} \mathbf{u}(\mathbf{R}) \mathbf{A}(\mathbf{R}-\mathbf{R}') \mathbf{u}(\mathbf{R}') \\
&\quad + \frac{1}{2} F''(\bar{\rho}) \sum_{\mathbf{R}} \left\{ \sum_{\mathbf{R}'} \mathbf{u}(\mathbf{R}') \rho_\mu(\mathbf{R}-\mathbf{R}') \right\} \left\{ \sum_{\mathbf{R}''} \rho_\nu(\mathbf{R}-\mathbf{R}'') \mathbf{u}(\mathbf{R}'') \right\}
\end{aligned} \tag{22}
$$

となる。さて、式(20)のフーリエ変換を計算してみよう。

$$
\begin{aligned}
A_{\mu\nu}(\mathbf{k}) &= \sum_{\mathbf{R}-\mathbf{R}'} A_{\mu\nu}(\mathbf{R}-\mathbf{R}') \exp\{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\} \\
&= \sum_{\mathbf{R}-\mathbf{R}'} \left\{ \begin{array}{l} \delta_{\mathbf{R}\mathbf{R}'} \sum_{\mathbf{R}''} \left[2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}'') + \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'') \right] \\ -2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}') - \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}') \end{array} \right\} \exp\{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\} \\
&= \sum_{\mathbf{R}} \left\{ \begin{array}{l} \delta_{\mathbf{R}} \sum_{\mathbf{R}''} \left[2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}'') + \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'') \right] \\ -2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}) - \phi_{\mu\nu}(\mathbf{R}) \end{array} \right\} \exp(-i\mathbf{k}\cdot\mathbf{R}) \\
&= \sum_{\mathbf{R}} \left\{ \delta_{\mathbf{R}} \sum_{\mathbf{R}''} \left[2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}'') + \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'') \right] \right\} \exp(-i\mathbf{k}\cdot\mathbf{R}) \\
&\quad - \sum_{\mathbf{R}} \left\{ 2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}) + \phi_{\mu\nu}(\mathbf{R}) \right\} \exp(-i\mathbf{k}\cdot\mathbf{R}) \\
&= \sum_{\mathbf{R}''} \sum_{\mathbf{R}} \left[2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}-\mathbf{R}'') + \phi_{\mu\nu}(\mathbf{R}-\mathbf{R}'') \right] \delta_{\mathbf{R}} \exp(-i\mathbf{k}\cdot\mathbf{R}) \\
&\quad - \sum_{\mathbf{R}} \left\{ 2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}) + \phi_{\mu\nu}(\mathbf{R}) \right\} \exp(-i\mathbf{k}\cdot\mathbf{R}) \\
&= \sum_{\mathbf{R}''} \left[2F'(\bar{\rho})\rho_{\mu\nu}(-\mathbf{R}'') + \phi_{\mu\nu}(-\mathbf{R}'') \right] - \sum_{\mathbf{R}} \left\{ 2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}) + \phi_{\mu\nu}(\mathbf{R}) \right\} \exp(-i\mathbf{k}\cdot\mathbf{R}) \\
&= \sum_{\mathbf{R}} \left[2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}) + \phi_{\mu\nu}(\mathbf{R}) \right] - \sum_{\mathbf{R}} \left\{ 2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}) + \phi_{\mu\nu}(\mathbf{R}) \right\} \exp(-i\mathbf{k}\cdot\mathbf{R}) \\
&= \sum_{\mathbf{R}} \left[2F'(\bar{\rho})\rho_{\mu\nu}(\mathbf{R}) + \phi_{\mu\nu}(\mathbf{R}) \right] \{1-\exp(-i\mathbf{k}\cdot\mathbf{R})\}
\end{aligned} \tag{23}
$$

となる。また、式(22)右辺第１項を逆空間で書き下すと、

$$
\begin{aligned}
&\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'} u_\mu(\mathbf{R})A_{\mu\nu}(\mathbf{R}-\mathbf{R}')u_\nu(\mathbf{R}') \\
&=\frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\left\{\sum_{\mathbf{k}} U_\mu(\mathbf{k})\exp(i\mathbf{k}\mathbf{R})\right\}\left\{\sum_{\mathbf{k}} A_{\mu\nu}(\mathbf{k})\exp\{i\mathbf{k}(\mathbf{R}-\mathbf{R}')\}\right\}\left\{\sum_{\mathbf{k}} U_\nu(\mathbf{k})\exp(i\mathbf{k}\mathbf{R}')\right\} \\
&=\frac{1}{2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{k}''} U_\mu(\mathbf{k}')U_\nu(\mathbf{k})A_{\mu\nu}(\mathbf{k}'')\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\exp(i\mathbf{k}'\mathbf{R})\exp(i\mathbf{k}\mathbf{R}')\exp\{i\mathbf{k}''(\mathbf{R}-\mathbf{R}')\} \qquad (24)\\
&=\frac{1}{2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{k}''} U_\mu(\mathbf{k}')U_\nu(\mathbf{k})A_{\mu\nu}(\mathbf{k}'')\sum_{\mathbf{R}}\exp\{i(\mathbf{k}'+\mathbf{k}'')\mathbf{R}\}\sum_{\mathbf{R}'}\exp\{i(\mathbf{k}-\mathbf{k}'')\mathbf{R}'\} \\
&=\frac{1}{2}\sum_{\mathbf{k}} A_{\mu\nu}(\mathbf{k})U_\mu(-\mathbf{k})U_\nu(\mathbf{k})
\end{aligned}
$$

を得る。次に、

$$
\begin{aligned}
&\rho_\mu(\mathbf{R}-\mathbf{R}')=\sum_{\mathbf{k}}\rho_\mu(\mathbf{k})\exp\{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')\} \\
&\rho_\mu(\mathbf{k})=\sum_{\mathbf{k}}\rho_\mu(\mathbf{R})\exp(-i\mathbf{k}\cdot\mathbf{R})
\end{aligned}
\qquad (25)
$$

と定義し、式(22)右辺第２項を逆空間で書き下すと、

$$
\begin{aligned}
&\frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{R}}\left\{\sum_{\mathbf{R}'}u_\mu(\mathbf{R}')\rho_\mu(\mathbf{R}-\mathbf{R}')\right\}\left\{\sum_{\mathbf{R}''}\rho_\nu(\mathbf{R}-\mathbf{R}'')u_\nu(\mathbf{R}'')\right\} \\
&=\frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{R}}\left[\begin{aligned}&\sum_{\mathbf{R}'}\left\{\sum_{\mathbf{k}}U_\mu(\mathbf{k})\exp(i\mathbf{k}\mathbf{R}')\right\}\left\{\sum_{\mathbf{k}}\rho_\mu(\mathbf{k})\exp\{i\mathbf{k}(\mathbf{R}-\mathbf{R}')\}\right\} \\ &\times\sum_{\mathbf{R}''}\left\{\sum_{\mathbf{k}}\rho_\nu(\mathbf{k})\exp\{i\mathbf{k}(\mathbf{R}-\mathbf{R}'')\}\right\}\left\{\sum_{\mathbf{k}}U_\nu(\mathbf{k})\exp(i\mathbf{k}\mathbf{R}'')\right\}\end{aligned}\right] \\
&=\frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{k}''}\sum_{\mathbf{k}'''}U_\mu(\mathbf{k})\rho_\mu(\mathbf{k}')\rho_\nu(\mathbf{k}'')U_\nu(\mathbf{k}''') \\
&\qquad\times\sum_{\mathbf{R}}\sum_{\mathbf{R}'}\sum_{\mathbf{R}''}\left[\begin{aligned}&\exp(i\mathbf{k}\mathbf{R}')\exp\{i\mathbf{k}'(\mathbf{R}-\mathbf{R}')\} \\ &\times\exp\{i\mathbf{k}''(\mathbf{R}-\mathbf{R}'')\}\exp(i\mathbf{k}'''\mathbf{R}'')\end{aligned}\right] \\
&=\frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{k}''}\sum_{\mathbf{k}'''}U_\mu(\mathbf{k})\rho_\mu(\mathbf{k}')\rho_\nu(\mathbf{k}'')U_\nu(\mathbf{k}''') \\
&\qquad\times\sum_{\mathbf{R}}\exp\{i(\mathbf{k}'+\mathbf{k}'')\mathbf{R})\}\sum_{\mathbf{R}'}\exp\{i(\mathbf{k}-\mathbf{k}')\mathbf{R}'\}\sum_{\mathbf{R}''}\exp\{i(\mathbf{k}'''-\mathbf{k}'')\mathbf{R}''\} \\
&=\frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{k}}U_\mu(\mathbf{k})\rho_\mu(\mathbf{k})\rho_\nu(-\mathbf{k})U_\nu(-\mathbf{k}) \\
&=\frac{1}{2}F''(\bar{\rho})\sum_{\mathbf{k}}U_\mu(-\mathbf{k})\rho_\mu(-\mathbf{k})\rho_\nu(\mathbf{k})U_\nu(\mathbf{k})
\end{aligned}
\qquad (26)
$$

となる。式(24)(26)より、式(22)の逆空間表示は、

$$
\begin{aligned}
E_D &= \frac{1}{2}\sum_{\mathbf{R},\mathbf{R}'} u_\mu(\mathbf{R}) A_{\mu\nu}(\mathbf{R}-\mathbf{R}') u_\nu(\mathbf{R}') \\
&\quad + \frac{1}{2} F''(\bar{\rho}) \sum_{\mathbf{R}} \left\{ \sum_{\mathbf{R}'} u_\mu(\mathbf{R}') \rho_\mu(\mathbf{R}-\mathbf{R}') \right\} \left\{ \sum_{\mathbf{R}''} \rho_\nu(\mathbf{R}-\mathbf{R}'') u_\nu(\mathbf{R}'') \right\} \\
&= \frac{1}{2}\sum_{\mathbf{k}} A_{\mu\nu}(\mathbf{k}) U_\mu(-\mathbf{k}) U_\nu(\mathbf{k}) + \frac{1}{2} F''(\bar{\rho}) \sum_{\mathbf{k}} U_\mu(-\mathbf{k}) \rho_\mu(-\mathbf{k}) \rho_\nu(\mathbf{k}) U_\nu(\mathbf{k}) \\
&= \frac{1}{2}\sum_{\mathbf{k}} U_\mu(-\mathbf{k}) \left[A_{\mu\nu}(\mathbf{k}) + F''(\bar{\rho}) \rho_\mu(-\mathbf{k}) \rho_\nu(\mathbf{k}) \right] U_\nu(\mathbf{k}) \\
&= \frac{1}{2}\sum_{\mathbf{k}} U_\mu(-\mathbf{k}) D_{\mu\nu}(\mathbf{k}) U_\nu(\mathbf{k})
\end{aligned}
\tag{27}
$$

にて与えられる。したがって、ダイナミカルマトリックスは、

$$
D_{\mu\nu}(\mathbf{k}) = A_{\mu\nu}(\mathbf{k}) + F''(\bar{\rho}) \rho_\mu(-\mathbf{k}) \rho_\nu(\mathbf{k}) \tag{28}
$$

にて定義される。

また、$A_{\mu\nu}(\mathbf{k}), \rho_\mu(\mathbf{k})$ を具体的に計算する際、

$$
\rho_\nu = \left(\frac{\partial \rho}{\partial R_\nu} \right) = \left(\frac{\partial \rho}{\partial R} \right) \frac{R_\nu}{R} = \rho' \frac{R_\nu}{R} \tag{29}
$$

$$
\begin{aligned}
\rho_{\mu\nu} &= \left(\frac{\partial^2 \rho}{\partial R_\mu \partial R_\nu} \right) = \frac{\partial}{\partial R_\mu} \left\{ \left(\frac{\partial \rho}{\partial R} \right) \frac{R_\nu}{R} \right\} = \left(\frac{\partial^2 \rho}{\partial R^2} \right) \frac{R_\mu R_\nu}{R^2} + \left(\frac{\partial \rho}{\partial R} \right) \left(\frac{\delta_{\mu\nu}}{R} - \frac{R_\mu R_\nu}{R^3} \right) \\
&= \left\{ \left(\frac{\partial^2 \rho}{\partial R^2} \right) - \frac{1}{R} \left(\frac{\partial \rho}{\partial R} \right) \right\} \frac{R_\mu R_\nu}{R^2} + \frac{\delta_{\mu\nu}}{R} \left(\frac{\partial \rho}{\partial R} \right) = \left\{ \rho'' - \frac{\rho'}{R} \right\} \frac{R_\mu R_\nu}{R^2} + \delta_{\mu\nu} \frac{\rho'}{R}
\end{aligned}
\tag{30}
$$

$$
\phi_\nu = \left(\frac{\partial \phi}{\partial R_\nu} \right) = \left(\frac{\partial \phi}{\partial R} \right) \frac{R_\nu}{R} = \phi' \frac{R_\nu}{R} \tag{31}
$$

$$
\begin{aligned}
\phi_{\mu\nu} &= \left(\frac{\partial^2 \phi}{\partial R_\mu \partial R_\nu} \right) = \frac{\partial}{\partial R_\mu} \left\{ \left(\frac{\partial \phi}{\partial R} \right) \frac{R_\nu}{R} \right\} = \left(\frac{\partial^2 \phi}{\partial R^2} \right) \frac{R_\mu R_\nu}{R^2} + \left(\frac{\partial \phi}{\partial R} \right) \left(\frac{\delta_{\mu\nu}}{R} - \frac{R_\mu R_\nu}{R^3} \right) \\
&= \left\{ \left(\frac{\partial^2 \phi}{\partial R^2} \right) - \frac{1}{R} \left(\frac{\partial \phi}{\partial R} \right) \right\} \frac{R_\mu R_\nu}{R^2} + \frac{\delta_{\mu\nu}}{R} \left(\frac{\partial \phi}{\partial R} \right) = \left\{ \phi'' - \frac{\phi'}{R} \right\} \frac{R_\mu R_\nu}{R^2} + \delta_{\mu\nu} \frac{\phi'}{R}
\end{aligned}
\tag{32}
$$

の関係が用いられる。式の変形において、$R^2 = R_1^2 + R_2^2 + R_3^2$ および $2RdR = 2R_i dR_i$ を用いた。これより、式(23)右辺の[ ]内は、

$$
\begin{aligned}
X_{\mu\nu}(\mathbf{R}) &\equiv \left[2F'(\bar{\rho}) \rho_{\mu\nu}(\mathbf{R}) + \phi_{\mu\nu}(\mathbf{R}) \right] \\
&= 2F'(\bar{\rho}) \left\{ \rho'' - \frac{\rho'}{R} \right\} \frac{R_\mu R_\nu}{R^2} + 2F'(\bar{\rho}) \delta_{\mu\nu} \frac{\rho'}{R} + \left\{ \phi'' - \frac{\phi'}{R} \right\} \frac{R_\mu R_\nu}{R^2} + \delta_{\mu\nu} \frac{\phi'}{R} \\
&= \left[\phi'' + 2F'(\bar{\rho}) \rho'' \right] \frac{R_\mu R_\nu}{R^2} + \left\{ \frac{\phi'}{R} + 2F'(\bar{\rho}) \frac{\rho'}{R} \right\} \left\{ \delta_{\mu\nu} - \frac{R_\mu R_\nu}{R^2} \right\}
\end{aligned}
\tag{33}
$$

となる。以上、ダイナミカルマトリックスに関してまとめると、

$$D_{\mu\nu}(\mathbf{k}) = A_{\mu\nu}(\mathbf{k}) + F''(\bar{\rho})\rho_\mu(-\mathbf{k})\rho_\nu(\mathbf{k})$$

$$A_{\mu\nu}(\mathbf{k}) = \sum_{\mathbf{R}} X_{\mu\nu}(\mathbf{R})\{1 - \exp(-i\mathbf{k}\cdot\mathbf{R})\}$$

$$X_{\mu\nu}(\mathbf{R}) = \left[\phi'' + 2F'(\bar{\rho})\rho''\right]\frac{R_\mu R_\nu}{R^2} + \left\{\frac{\phi'}{R} + 2F'(\bar{\rho})\frac{\rho'}{R}\right\}\left(\delta_{\mu\nu} - \frac{R_\mu R_\nu}{R^2}\right)$$

$$\rho_\mu(\mathbf{k}) = \sum_{\mathbf{R}} \rho_\mu(\mathbf{R})\exp(-i\mathbf{k}\cdot\mathbf{R})$$

$$\rho_\mu(\mathbf{R}) = \rho'\frac{R_\mu}{R}$$

$$F''(\bar{\rho}) = \left(\frac{\partial^2 F}{\partial\bar{\rho}^2}\right) \quad , \quad F'(\bar{\rho}) = \left(\frac{\partial F}{\partial\bar{\rho}}\right)$$

$$\phi'' = \left(\frac{\partial^2\phi}{\partial R^2}\right) \quad , \quad \phi' = \left(\frac{\partial\phi}{\partial R}\right) \quad , \quad \rho'' = \left(\frac{\partial^2\rho}{\partial R^2}\right) \quad , \quad \rho' = \left(\frac{\partial\rho}{\partial R}\right) \quad , \quad R^2 = R_1^2 + R_2^2 + R_3^2$$

となる。マトリックス表記すれば、

$$\mathbf{D}(\mathbf{k}) = \mathbf{A}(\mathbf{k}) + F''(\bar{\rho})\underline{\rho}(-\mathbf{k})\underline{\rho}(\mathbf{k})$$

$$\mathbf{A}(\mathbf{k}) = \sum_{\mathbf{R}} \mathbf{X}(\mathbf{R})\{1 - \exp(-i\mathbf{k}\cdot\mathbf{R})\}$$

RR

$$\mathbf{X}(\mathbf{R}) = \left[\phi'' + 2F'(\bar{\rho})\rho''\right]\frac{\mathbf{RR}}{R^2} + \left\{\frac{\phi'}{R} + 2F'(\bar{\rho})\frac{\rho'}{R}\right\}\left(\mathbf{1} - \frac{\mathbf{RR}}{R^2}\right)$$

（注：**RR** はベクトルの通常の積あり、内積ではない。）

$$\underline{\rho}(\mathbf{k}) = \sum_{\mathbf{R}} \underline{\rho}(\mathbf{R})\exp(-i\mathbf{k}\cdot\mathbf{R})$$

$$\underline{\rho}(\mathbf{R}) = \rho'\frac{\mathbf{R}}{R}$$

$$F''(\bar{\rho}) = \left(\frac{\partial^2 F}{\partial\bar{\rho}^2}\right) \quad , \quad F'(\bar{\rho}) = \left(\frac{\partial F}{\partial\bar{\rho}}\right)$$

$$\phi'' = \left(\frac{\partial^2\phi}{\partial R^2}\right) \quad , \quad \phi' = \left(\frac{\partial\phi}{\partial R}\right)$$

$$\rho'' = \left(\frac{\partial^2\rho}{\partial R^2}\right) \quad , \quad \rho' = \left(\frac{\partial\rho}{\partial R}\right) \quad , \quad |\mathbf{R}|^2 = R^2 = R_1^2 + R_2^2 + R_3^2$$

である。