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ERROR ESTIMATE OF FORCE-BASED QUASICONTINUUM METHOD*

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Abstract. We prove that the force-based quasicontinuum method converges uniformly with first order accuracy.

Key words. Quasicontinuum method, ghost force, convergence, accuracy

AMS subject classifications. 65N30, 65N06, 74G20

1. Introduction

The quasicontinuum (QC) [30] method is among the most successful multiscale methods for modeling the mechanical deformation of solids. So far, its main success is in modeling the static properties of crystalline solids at zero temperature. At the same time, QC has attracted a great deal of attention from the numerical analysis community since it provides the simplest example for understanding the algorithmic issues in coupled atomistic-continuum methods [1, 2, 5, 6, 10, 18, 19, 22, 24]. At zero temperature, the atomistic model can be regarded as a consistent discretization of the Cauchy-Born continuum model whenever the system is in the elastic regime [7, 8]. Since QC uses the Cauchy-Born rule in the continuum region (or the local region, in the QC terminology), the models used in the continuum and atomistic regions (or local and nonlocal regions) are consistent. The only remaining issue is what happens at the interface when the two models couple. Indeed, errors are introduced by QC at the interface. The simplest and most well-known issue is the "ghost force" [26], i.e., forces that act on the atoms when they are in equilibrium positions. Since the forces acting on atoms should vanish when they are in equilibrium positions, whatever forces are present are due to numerical error. There are several ways to remove the ghost force; among them the simplest is the force-based QC [26, 20, 21]. Dobson and Luskin [2] have shown the convergence of the iterations for this version of QC. We shall prove the uniform first order convergence of force-based QC in this note, and refer to [10] for the analysis of other versions of QC [28, 4].

Following [10], we view the interface as an internal numerical boundary where two different numerical schemes meet. Both are consistent with the underlying PDE, in this case, the Cauchy-Born elasticity model. We will show in this note and the follow-up paper [22] that the accuracy and stability issues in QC can be understood by following standard practices in classical numerical analysis.

A brief outline of this note is as follows. In §2, we will introduce QC and the force-based QC, and we then show by a simple example the structure of the error caused by the ghost force. In §3, we will see that even though the local truncation error (LTE) is $\mathcal{O}(1)$, it is of divergence form and is actually $\mathcal{O}(\epsilon)$ in a weak norm, for example the so-called *Spijker norm* [31, 29], where ϵ is the equilibrium bond length.

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We then show that the stability condition and the LTE analysis imply that the force-based QC recovers uniform first order accuracy. Our strategy closely follows that of [10].

2. The quasicontinuum method

We will consider a one-dimensional chain with $2N+1$ atoms, indexed by $-N,\dots,N$, interacting with a two-body potential V_0 that depends on the distance between the atoms, with some additional boundary atoms which are fixed at their equilibrium positions:

$$y_i^\epsilon = i\epsilon, \qquad i = N+1, N+2, -N-1, -N-2. \tag{2.1}$$

Here ϵ is the equilibrium bond length and we assume that $2N\epsilon = 1$. Let $\bar{r} = r/\epsilon$, and rescale the potential function V_0 as $V(\bar{r}) = V_0(r)$. We always assume that

$$V''(1) > 7|V''(2)|. \tag{2.2}$$

We will only consider the case of next nearest neighbor interaction. This is the simplest case when QC is non-trivial, i.e., it does not coincide with the full atomistic model. It will be clear from the presentation that similar analysis carries over to the case of any finite range interaction [9].

By (2.1), we define the admissible set for the solution by

$$\mathcal{S} = \{\, \boldsymbol{z} \in \mathbb{R}^{2N+5} \mid z_i = i\epsilon, \quad i = N+1, N+2, -N-1, -N-2 \,\}.$$

Given the external force $\boldsymbol{f} = (f_{-N}, \dots, f_N)$, the atomistic problem we need to solve is: find $\boldsymbol{y}^\epsilon \in \mathcal{S}$ that satisfies

$$\mathcal{L}^\epsilon_{\text{atom}}(\boldsymbol{y}^\epsilon) = \boldsymbol{f}. \tag{2.3}$$

We write (2.3) in component form as, for $i = -N, \dots, N$,

$$-\frac{1}{\epsilon}\Big\{ V'(D^+ y_{i-1}) + V'(2\widehat{D} y_{i-1}) + V'(-D^+ y_i) + V'(-2\widehat{D} y_{i+1}) \Big\} = f_i, \tag{2.4}$$

where $D^+ y_i = (y_{i+1} - y_i)/\epsilon, D^- y_i = (y_i - y_{i-1})/\epsilon$ and $\widehat{D} = (D^+ + D^-)/2$. Using the fact that V' is an odd function, we may write (2.4) into a more compact form:

$$D^- V'(D^+ y_i) + 2\widehat{D} V'(2\widehat{D} y_i) = f_i.$$

We assume that there exists a smooth function $f(x) : [-1/2, 1/2] \to \mathbb{R}$ such that

$$f(x_i) = f_i, \quad x_i = i\epsilon, i = -N, \dots, N, \tag{2.5}$$

where f_i is the external force acting on the i-th atom.

For the solution $\boldsymbol{y}^\epsilon$ of the atomistic model, we have the following existence result and a priori estimate [10, Lem. 5.6].

LEMMA 2.1. *If the stability condition* (2.2) *holds, then for $p \geq 1$ there exists a constant δ such that if $\|f\|_{W^{4,p}(0,L)} \leq \delta$, the problem* (2.3) *has one and only one solution $\boldsymbol{y}^\epsilon \in \mathcal{S}$. Moreover, we have the following a priori estimate for $\boldsymbol{y}^\epsilon$. For i=-N+3,. . . ,N-3, the following holds.*

$$\sum_{k=1}^{3} \|(D^+)^k y_i^\epsilon\|_\infty \leq C. \tag{2.6}$$

2.1. Ghost force in QC. The first step in QC is coarse-graining, i.e., selecting representative atoms. Since we are focusing on the interface between the continuum and atomistic regions, we will consider the case when every atom is a representative atom. The first N atoms, indexed by $j=-N,\dots,-1$, will make up the nonlocal region in which the original atomistic model will be used. The atoms indexed by $j=1,\dots,N$ will make the local region in which the Cauchy-Born continuum model will be used. The atom indexed by 0 separates the two regions. We shall use $\bar{i}$ to replace $-i$ in certain situations. The equilibrium equations for the atoms indexed by $-N,\dots,-2$ are the same as (2.4). For atoms indexed by $2,\dots,N$, we have

$$\mathcal{L}^{\epsilon}_{\rm cb}(\boldsymbol{y})_i = f_i,$$

where

$$\mathcal{L}^{\epsilon}_{\rm cb}(\boldsymbol{y})_i = -\frac{1}{\epsilon}\big\{V'(D^+y_{i-1})+V'(-D^+y_i)+2V'(2D^+y_{i-1})+2V'(-2D^+y_i)\big\}.$$

The equilibrium equations for the interfacial atoms $\bar{1}$,0 and 1 are:

$$\begin{aligned}
-\frac{1}{\epsilon}\left\{V'(2\widehat{D}y_{\bar{2}})+V'(D^+y_{\bar{2}})+V'(-D^+y_{\bar{1}})+\frac{1}{2}V'(-2\widehat{D}y_0)\right\} &= f_{\bar{1}},\\
-\frac{1}{\epsilon}\left\{V'(2\widehat{D}y_{\bar{1}})+V'(D^+y_{\bar{1}})+V'(-D^+y_0)+2V'(-2D^+y_0)\right\} &= f_0,\\
-\frac{1}{\epsilon}\left\{\frac{1}{2}V'(2\widehat{D}y_0)+V'(D^+y_0)+V'(-D^+y_1)+2V'(2D^+y_0)+2V'(-2D^+y_1)\right\} &= f_1.
\end{aligned}$$

We will write these equations in a compact form as

$$\mathcal{L}^{\epsilon}_{\rm qc}(\boldsymbol{y}) = \boldsymbol{f}. \tag{2.7}$$

To calculate the ghost force, recall that the undeformed state is $\boldsymbol{x}=(x_{-N},\cdots,x_N)$ with $x_i=i\epsilon$. It is obvious that

$$\mathcal{L}^{\epsilon}_{\rm atom}(\boldsymbol{x})=\boldsymbol{0} \quad \text{and} \quad \mathcal{L}^{\epsilon}_{\rm cb}(\boldsymbol{x})=\boldsymbol{0}.$$

However, a direct calculation gives

$$\mathcal{L}^{\epsilon}_{\rm qc}(\boldsymbol{x})_{\bar{1}} = -\frac{V'(2)}{2\epsilon}, \quad \mathcal{L}^{\epsilon}_{\rm qc}(\boldsymbol{x})_0 = \frac{V'(2)}{\epsilon}, \quad \mathcal{L}^{\epsilon}_{\rm qc}(\boldsymbol{x})_1 = -\frac{V'(2)}{2\epsilon}.$$

This is called the ghost-force.

To see explicitly the error induced by the ghost force, we consider a one-dimensional chain interacted with the harmonic potential

$$V(x_1,x_2)=\frac{1}{2}\left(\frac{x_1-x_2}{\epsilon}\right)^2.$$

In the absence of the external force, the atom is in equilibrium, therefore, $\boldsymbol{y}^{\epsilon}=\boldsymbol{x}$.

THEOREM 2.1. *[10, Thm. 3.1] Let $\boldsymbol{y}$ be the solution of (2.7). Then,*

$$\begin{aligned}
&|D^+(y_i-x_i)| \le C\left(\epsilon+\left|\frac{3-\sqrt{5}}{2}\right|^{-i}\right), \qquad i=-N,\dots,0,\\
&|D^+(y_i-x_i)| \le C\epsilon, \qquad i=1,\dots,N.
\end{aligned} \tag{2.8}$$

Moreover, we have

$$D^+(y_0-x_0)\geq \frac{9(\sqrt{5}-1)}{17+5\sqrt{5}},\qquad N\geq 4. \tag{2.9}$$

A direct corollary of the above result is the characterization of the width of the interface, that is, the region beyond which $|D^+(\boldsymbol{y}-\boldsymbol{x})|=\mathcal{O}(\epsilon)$.

COROLLARY 2.2. *Let* $\boldsymbol{y}$ *be the solution of* (2.7). *The following holds:*

$$|D^+(y_i-x_i)|\leq C\epsilon,\qquad i=-N,\ldots,-\left\lceil\left|\frac{\ln\epsilon}{\ln(3+\sqrt{5})/2}\right|\right\rceil \quad or \quad i=1,\ldots,N.$$

REMARK 2.3. Since the lattice constant is $\mathcal{O}(\epsilon)$, we see that the width of the interface is $\mathcal{O}(\epsilon|\ln\epsilon|)$. A similar result has also been proved by Dobson and Luskin in [3] for a quadratic potential obtained by linearizing around the equilibrium state of a pairwise potential.

The simplest idea for removing the ghost force is a force-based approach [26, 20, 21]. Similar ideas may be found in [14, 12, 27]. In this approach, one defines

$$(\mathcal{L}^\epsilon_{\rm fqc})_i=\begin{cases}(\mathcal{L}^\epsilon_{\rm atom})_i & \text{if} \quad -N\leq i\leq 0,\\ (\mathcal{L}^\epsilon_{\rm cb})_i & \text{if} \quad 1\leq i\leq N.\end{cases}$$

The deformed positions of the atoms are found by solving

$$\mathcal{L}^\epsilon_{\rm fqc}(\boldsymbol{y})=\boldsymbol{f} \tag{2.10}$$

with the same boundary condition (2.1).

Obviously, $\mathcal{L}^\epsilon_{\rm fqc}(\boldsymbol{x})=\boldsymbol{0}$, therefore, the force-based QC is free of ghost force.

There are other approaches to remove the ghost force, for example, the quasi-nonlocal QC introduced by Shimokawa et al [28] and the geometrically consistent scheme proposed by E et al. [4]. In contrast to force-based QC, both schemes have a well-defined total energy. We refer to [10] for the analysis of such methods.

3. Error estimates of the force-based QC

To analyze the accuracy of force-based QC, we follow the strategy in [10]. To avoid the influence of the boundary condition [32], we simply let

$$(\mathcal{L}^\epsilon_{\rm fqc})_i=(\mathcal{L}^\epsilon_{\rm atom})_i,\quad i=N-1,N.$$

We define the truncation error functional as $\boldsymbol{F}=(\mathcal{L}^\epsilon_{\rm atom}-\mathcal{L}^\epsilon_{\rm fqc})(\boldsymbol{y}^\epsilon)$. A Taylor expansion gives

$$\begin{aligned}&F_k=0,\quad k=-N,\ldots,-1,N-1,N,\\ &F_k=f_k-\int_0^1\Big[V''\big(tD^+y^\epsilon_k+(1-t)D^+y^\epsilon_{k-1}\big)\\ &\qquad\qquad +4V''\big(2tD^+y^\epsilon_k+2(1-t)D^+y^\epsilon_{k-1}\big)\Big]{\rm d}t\cdot(D^+)^2y^\epsilon_{k-1},\quad k=0,\ldots,N-2.\end{aligned}$$

In view of (2.6) and the above equations, we have

$$\boldsymbol{F}=\mathcal{O}(1), \tag{3.1}$$

which seems to suggest that this scheme does not converge. However, as noted in [10], the truncation error has some structure that can be exploited due to the translation invariance of the potential function [15] and the periodicity of the underlying lattice structure [25]. For $k=-N,\dots,-1,N-1,N$, $F_k=0$, while for $k=0,\cdots,N-2$, we have

$$\begin{cases} F_k=D^+Q_k, \\ Q_k=V'(2\widehat{D}y_k)+V'(2\widehat{D}y_{k-1})-2V'(2D^+y_{k-1}). \end{cases} \tag{3.2}$$

We will see in the following lemma that $Q=\mathcal{O}(\epsilon^2)$. In what follows, we denote by $\langle\cdot,\cdot\rangle$ the standard inner product.

LEMMA 3.1. *For $\boldsymbol{w}\in\mathbb{R}^{2N+1}$, we have*

$$|\langle\boldsymbol{F},\boldsymbol{w}\rangle|\le C\epsilon\|\boldsymbol{w}\|_d, \tag{3.3}$$

where $\|\boldsymbol{w}\|_d=\left(\epsilon^{-2}(w_{-N}^2+w_N^2)+\sum_{i=-N}^{N-1}|D^+w_i|^2\right)^{1/2}$.

Proof. Using (3.2) and summation by parts we have

$$\begin{aligned}\langle\boldsymbol{F},\boldsymbol{w}\rangle=\sum_{k=-N}^{N}F_kw_k=\sum_{k=0}^{N-2}F_kw_k=\sum_{k=0}^{N-2}D^+Q_kw_k \\ =-\sum_{k=0}^{N-3}Q_{k+1}D^+w_k-Q_0\frac{w_0}{\epsilon}+Q_{N-1}\frac{w_{N-2}}{\epsilon}.\end{aligned} \tag{3.4}$$

Using a Taylor expansion, we can write Q_k for $k=0,\cdots,N-1$ as

$$\begin{aligned}Q_k=&\epsilon\left[\int_0^1V''\big(2+(1+t)D^+\hat{y}_{k-1}+(1-t)D^+\hat{y}_k\big)\mathrm{d}t\right](D^+)^2\hat{y}_{k-1}\\&-\epsilon\left[\int_0^1V''\big(2+(1+t)D^+\hat{y}_{k-1}+(1-t)D^+\hat{y}_{k-2}\big)\mathrm{d}t\right](D^+)^2\hat{y}_{k-2}\\=&\epsilon^2\left[\int_0^1V''\big(2+(1+t)D^+\hat{y}_{k-1}+(1-t)D^+\hat{y}_k\big)\mathrm{d}t\right](D^+)^3\hat{y}_{k-2}\\&-\epsilon^2\left[\int_0^1\int_0^1V'''\big(2+(1+t)D^+\hat{y}_{k-1}+(1-t)D^+(s\hat{y}_k+(1-s)\hat{y}_{k-2})\big)\mathrm{d}s\mathrm{d}t\right]\\&\times(D^+)^2(\hat{y}_{k-2}+\hat{y}_{k-1})(D^+)^2\hat{y}_{k-2}.\end{aligned}$$

Using (2.6), the discrete Wirtinger inequality [11, Thm. 9],

$$\epsilon^{1/2}\max_{-N\le i\le N}|w_i|\le\left(\sum_{i=-N}^{N}\epsilon w_i^2\right)^{1/2}\le\epsilon^{1/2}\frac{N+1}{2N}\|\boldsymbol{w}\|_d\le\epsilon^{1/2}\|\boldsymbol{z}\|_d, \tag{3.5}$$

and the identity above, we obtain

$$|\langle\boldsymbol{F},\boldsymbol{w}\rangle|\le C\left(\epsilon^2\sum_{k=1}^{N-1}|D^+w_k|+\epsilon|w_0|+\epsilon^2\|\boldsymbol{w}\|_d\right)\le C(\epsilon^{3/2}+\epsilon+\epsilon^2)\|\boldsymbol{w}\|_d\le C\epsilon\|\boldsymbol{w}\|_d.\ \square$$

Next we turn to the stability of the force-based QC. Since there is no well-defined energy functional for the force-based QC, the Hessian matrix $\mathcal{H}_{\rm fqc}$ is defined as

$$H_{i,j}=-\frac{\partial(\mathcal{L}^{\epsilon}_{\rm fqc})_i}{\partial w_j}(\boldsymbol{w}),\qquad i,j=-N,\dots,N,$$

where $\mathcal{L}^{\epsilon}_{\rm fqc}$ is regarded as a function of $\boldsymbol{w}$. By the following elementary identity:

$$a^2-ab=\frac{1}{2}(a-b)^2+\frac{1}{2}a^2-\frac{1}{2}b^2,\quad a,b\in\mathbb{R},$$

a direct calculation gives, for any $\boldsymbol{z}\in\mathbb{R}^{2N}$,

$$\begin{aligned}\epsilon^2\langle\mathcal{H}_{\rm fqc}(\boldsymbol{x})\boldsymbol{z},\boldsymbol{z}\rangle=&[V''(1)+V''(2)]z_{-N}^2+V''(2)z_{-N+1}^2+\left(V''(1)+\frac{3}{2}V''(2)\right)z_N^2\\&+V''(1)\left(\sum_{i=-N}^{-2}|z_i-z_{i+1}|^2+|z_{N-1}-z_N|^2\right)\\&+[V''(1)+4V''(2)]\sum_{i=0}^{N-3}|z_i-z_{i+1}|^2\\&+[V''(1)+2V''(2)](|z_{\bar1}-z_0|^2+|z_{N-2}-z_{N-1}|^2)\\&+V''(2)\left(\sum_{i=-N}^{-3}|z_i-z_{i+2}|^2+\frac{1}{2}\sum_{\substack{i=\bar2,\bar1\\ i=N-3,N-2}}|z_i-z_{i+2}|^2\right)\\&+\frac{V''(2)}{2}(z_{\bar2}^2+3z_{\bar0}^2+3z_{N-2}^2)-\frac{V''(2)}{2}(z_{\bar1}^2+z_{\bar1}^2+z_{N-1}^2+z_{N-3}^2).\end{aligned}\tag{3.6}$$

LEMMA 3.2. *For any $\boldsymbol{z}\in\mathbb{R}^{2N}$, the following holds.*

$$\langle\mathcal{H}_{fqc}(\boldsymbol{x})\boldsymbol{z},\boldsymbol{z}\rangle\ge\big(V''(1)-7|V''(2)|\big)\|\boldsymbol{z}\|_d^2,\quad N\ge4.\tag{3.7}$$

Proof. We start with (3.6). If $V''(2)<0$, then by Cauchy-Schwartz inequality:

$$|z_i-z_{i+2}|^2\le2(|z_i-z_{i+1}|^2+|z_{i+1}-z_{i+2}|^2),$$

and we write (3.6) as

$$\begin{aligned}\epsilon^2\langle\mathcal{H}_{\rm fqc}(\boldsymbol{x})\boldsymbol{z},\boldsymbol{z}\rangle\ge&\Big([V''(1)+V''(2)]z_{-N}^2+[V''(1)+2V''(2)]|z_{-N}-z_{-N+1}|^2\\&+V''(2)z_{-N+1}^2\Big)+[V''(1)+5V''(2)]\sum_{i=-N+1}^{N-1}|z_i-z_{i+1}|^2\\&+\left(V''(1)+\frac{3}{2}V''(2)\right)z_N^2+\frac{V''(2)}{2}(z_{\bar2}^2+3z_{\bar0}^2+3z_{N-2}^2).\end{aligned}$$

Note that

$$\begin{aligned}&[V''(1)+V''(2)]z_{-N}^2+V''(2)z_{-N+1}^2+[V''(1)+2V''(2)]|z_{-N}-z_{-N+1}|^2\\=&[V''(1)+4V''(2)](z_{-N}^2+|z_{-N}-z_{-N+1}|^2)\\&+|V''(2)|[z_{-N}^2+(2z_{-N}-z_{-N+1})^2].\end{aligned}$$

Using the discrete Wirtinger inequality (3.5), we have

$$\frac{V''(2)}{2}(z_2^2+3z_0^2+3z_{N-2}^2)\geq\frac{7V''(2)}{2}\left(\frac{N+1}{2N}\right)^2\|\boldsymbol{z}\|_d^2\geq 2\|\boldsymbol{z}\|_d^2.$$

Combining the above three inequalities gives (3.7).

If $V''(2)>0$, it follows from (3.6) that

$$\epsilon^2\langle\mathcal{H}_{\rm fqc}(\boldsymbol{x})\boldsymbol{z},\boldsymbol{z}\rangle\geq V''(1)\|\boldsymbol{z}\|_d^2-\frac{V''(2)}{2}(z_1^2+z_1^2+z_{N-1}^2+z_{N-3}^2),$$

and using the discrete Wirtinger inequality (3.5) once again, we obtain,

$$\epsilon^2\langle\mathcal{H}_{\rm fqc}(\boldsymbol{x})\boldsymbol{z},\boldsymbol{z}\rangle\geq(V''(1)-2V''(2))\|\boldsymbol{z}\|_d^2,$$

which gives (3.7). ∎

Following the same approach as [10, Thm. 5.16] which is mainly a fixed-point argument, we have the main result.

THEOREM 3.1. *If $p\geq 1, m\geq 4$, then there exists a constant κ such that if $\|\boldsymbol{f}\|_{W^{m,p}(0,L)}\leq\kappa$ and the stability condition (2.2) holds, then the problem (2.10) has one and only one solution $\boldsymbol{y}_{fqc}\in\mathcal{S}$. Moreover, $\boldsymbol{y}_{fqc}$ satisfies*

$$\|D^+(\boldsymbol{y}_{fqc}-\boldsymbol{y}^\epsilon)\|_\infty\leq C\epsilon. \tag{3.8}$$

REMARK 3.2. The uniform first order convergence of the force-based QC seems quite unexpected since (3.1) suggests that the local truncation error of such a scheme is $\mathcal{O}(1)$. The origin of the above result lies in the *supra-convergence* phenomenon [16, 31] as shown in Lemma 3.1.

Finally part we verify the stability condition (2.2) for several pairwise potentials.

First we consider the Lennard-Jones potential [17]:

$$V_0(r)=4\big((\sigma/r)^{12}-(\sigma/r)^6\big),$$

where σ is some atomic length scale parameter. The equilibrium bond length $\epsilon=(2/K)^{1/6}\sigma$ with $K=(1+2^{-6})/(1+2^{-12})>1$. A direct calculation gives

$$V''(2)<0\quad\text{and}\quad V''(1)-7|V''(2)|=V''(1)+7V''(2)>72K>0.$$

This verifies (2.2).

The next example is the Morse potential [23]:

$$V_0(r)=e^{-2a(r-r_0)}-2e^{-a(r-r_0)},$$

where a is a constant with dimension of the reciprocal of distance, and r_0 is the atomic length scale parameter. Let ϵ be the equilibrium bond length and denote by $s=e^{ar_0}$ and $t=e^{-a\epsilon}$. We find that t satisfies

$$2st^3+(s-2)t-1=0. \tag{3.9}$$

It is clear to see that there exists a unique solution $t\in(0,1)$, denoted by t_0,

$$V''(1)-7|V''(2)|=2a^2\epsilon^2st_0(2st_0-1-7|1+t_0-st_0|).$$

Metal	Rb	Cs	Na	K	Ba	Fe	Cr
ar_0	1.206	1.260	1.267	1.293	1.650	1.988	2.260
M	1.407	1.575	1.596	1.669	1.112	.863	.815
$\mathrm{sgn}(V''(2))$	+	+	+	+	−	−	−

TABLE 3.1. *Parameters for various metal; data for ar_0 adopted from [Table I] [13]*

Let $M := 2st_0 - 1 - 7|1 + t_0 - st_0|$. For the cubic metals listed in [13], e.g., Rb, Cs, Na, K, Ba, Fe, Cr, et al., see Table 3.1 for the corresponding values of M.

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