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On the "Preconditioning" Function Used in Planewave DFT Calculations and its Generalization

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Abstract. The Teter, Payne, and Allan "preconditioning" function plays a significant role in planewave DFT calculations. This function is often called the TPA preconditioner. We present a detailed study of this "preconditioning" function. We develop a general formula that can readily generate a class of "preconditioning" functions. These functions have higher order approximation accuracy and fulfill the two essential "preconditioning" purposes as required in planewave DFT calculations. Our general class of functions are expected to have applications in other areas.

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1 Introduction

Density functional theory (DFT) [6, 9] has profound impacts on atomic scale material studies, including materials processing and design. There are now quite extensive literature on DFT. Readers interested in the role of DFT within molecular and condensed matter physics may consult a few recent books *e.g.* [3, 8, 12, 15].

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One major approach for DFT calculations is by using planewave basis expansion. There are several influential planewave DFT software, including the open source QUANTUM- ESPRESSO [4,18], ABINIT [5,17], and the commercial VASP [10,19]. Readers interested in learning planewave DFT calculations may start with the nice KSSOLV package written in Matlab [21].

In DFT calculations for atomic scale study of materials, the major computational cost is usually spent on solving the Kohn-Sham equation. This equation is a nonlinear eigenvalue problem, which represents certain simplification of the Schrödinger equation to make it more numerically tractable. A self-consistency loop is utilized to address the nonlinearity, which means a sequence of linearized eigenvalue problems need to be solved until self-consistency is reached [12, 15]. Therefore, eigensolvers used in the DFT packages can be of crucial importance for the efficiency of the DFT calculations.

For the planewave DFT packages ([4,5,10,21] and others), two of the essential eigensolvers implemented are the preconditioned CG method and the preconditioned Davidson method. The efficiency of these eigensolvers is closely related to the following "preconditioning" function,

$$K(x)=\frac{27+18x+12x^2+8x^3}{27+18x+12x^2+8x^3+16x^4}. \tag{1.1}$$

However, few studies of this function appear in the planewave DFT literature, except that most papers utilizing a preconditioned eigensolver in the planewave setting would refer to the work of Teter, Payne and Allan [16]. The function $K(x)$ was first proposed in [16] and is now known as the TPA preconditioner.

A known property of $K(x)$ is that its derivatives up to order 3 at $x=0$ are all zeros. At first sight the $K(x)$ appears intriguing. One may wonder why $K(x)$ has to be in the form (1.1). Do the coefficients as listed in (1.1) lead to the property that $K'(0)=K''(0)=K'''(0)=0$? Can the coefficients be modified?

In this note we develop a generalization of $K(x)$. Besides readily answering the previously mentioned questions about $K(x)$, our generalization provides formulas with higher accuracy to fulfill the purposes of "preconditioning" in the planewave setting.

2 Up to order n consecutive zero derivatives at $x=0$

Our first finding is that there is no particular mystery related to $K'(0)=K''(0)=K'''(0)=0$, this property actually is independent of the coefficients listed in (1.1). In fact, it is a special case of the general result we present below.

We first define $p_n(x)$ and $g_n(x)$ as

$$p_n(x):=c_0+c_1x+c_2x^2+\cdots+c_nx^n, \tag{2.1}$$

$$g_n(x):=\frac{p_n(x)}{p_n(x)+c_{n+1}x^{n+1}}. \tag{2.2}$$