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Principles of the Theory of Lattice Dynamics

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Dedicated to Professor O. Stasiw

PREFACE

Much progress has been made during the last two decades in the theoretical understanding of dynamical properties of solids, especially of disordered and anharmonic solids. This progress is based on the application of new effective analytical and numerical methods, such as the Green function method and the molecular dynamics technique. The Green function method, for example, renders it possible to study solids with arbitrary defect concentrations and even, with fair success, to study solids with glass-like disorder. The Green function method is also a powerful tool for investigating anharmonic solids, including strongly anharmonic solids which cannot be treated by perturbation theory.

Among the problems of lattice dynamics having attracted particular interest in recent years are dynamical properties of disordered solids (localization of vibrational states, breakdown of quasi-momentum selection rules, role of short-range order) and anharmonic solids (strong anharmonicity, phonon hydrodynamics), dynamical aspects of anharmonicity and electron-phonon driven phase transitions (phonon softening, lattice solitons) and the development of a microscopic theory of lattice dynamics.

On a 'quick trip through lattice dynamics' I present here basic ideas and theoretical methods which have been developed in recent years for describing dynamical properties of solids, in particular, of disordered and anharmonic solids. I hope that this book will help the researcher in lattice dynamics to make himself acquainted with recent advances in fields which are somewhat remote from his special field of research. But I believe that the present book may also serve as introductory textbook to the theory of lattice vibrations. To a large extent, the book is based on lectures I gave for advanced students from 1972 to 1979 in Berlin at the Humboldt University.

Chapter 1 contains a concise compilation of basic elements of the theory of lattice dynamics knowledge of which is a necessary prerequisite for an understanding of the following chapters. This chapter also contains the microscopic approach to lattice dynamics which is based on a study of the response of the crystal electrons to the field produced by the vibrating ions (dielectric function approach).

Chapter 2 is devoted to compositionally disordered systems, including solids with single isolated defects. In this chapter the main emphasis is on the introduction of the Green function technique and on the use of this technique for evaluating configuration averaged quantities.

Chapter 3 is devoted to structurally disordered systems. Using the Green function method, in this chapter the problem of localized and plane-wave-like states is studied. Owing to the lack of a periodic reference lattice, the investigation of structurally disordered solids turns out to be in general much more complicated than that of compositionally disordered solids.

Chapter 4 is devoted to anharmonic systems and systems exhibiting structural phase transitions. Perturbation theory is developed for weakly anharmonic solids, and a self-consistent harmonic approximation for strongly anharmonic solids. Further topics treated in this chapter are lattice solitons, the Peierls transition and incommensurate structures.

Some topics with more formal character (application of group theory to lattice dynamics, response of crystal electrons to an electromagnetic field, calculation of experimental quantities) are given in the appendix.

It should be noted that in order to bring this book up-to-date I also included some problems (such as phonon-like excitations in structurally disordered solids, certain problems of incommensurate systems, etc.) where no full consensus is evident from present literature. Furthermore, the choice of the material presented here is to some extent arbitrary. Some fields (such as vibrational properties of surfaces, interaction of phonons with other elementary excitations, etc.) I have completely ignored.

The list of references is not complete. It contains, above all, only review articles and more recent original papers.

This book was written while I was at the Zentralinstitut für Elektronenphysik of the Academy of Sciences of the GDR in Berlin. I would like to thank my former colleagues Dr. M. Giehler, Dr. E. Jahne, Dr. P. Kleinert, R. Leihkauf, Dr. W. Ulrici and Dr. D. Wruck for helpful conversations. Furthermore, I am indepted to Prof. W. Kuhn for valuable suggestions, to Dr. T. Nattermann for critical remarks concerning section 4.4., to B. Gärtner for critically reading the manuscript, and to Mrs. Trautmann, Akademie-Verlag, for efficient cooperation. Finally, I wish to thank my wife who gave me enormous help with the preparation of the manuscript.

H. Böttger

CONTENTS

CHAPTER 1
BASIC ELEMENTS OF THE THEORIE OF LATTICE DYNAMICS

This chapter is an introductory one. We summarize here some elements of the theory of lattice dynamics which will be needed in the following chapters. We describe the phenomenological approach to lattice dynamics[1]. This approach is based on the idea that the motion of the atoms in a solid is governed by force constants which may be regarded as parameters resulting from experimental data. Furthermore, we outline the microscopic approach to lattice dynamics. This approach is based on a microscopic examination of the forces between the ions. It provides a useful tool for studying the relationship between the different force constant models used in the phenomenological theory of lattice dynamics.

1.1. The adiabatic approximation

According to Born and Oppenheimer in a solid the dynamical aspects of nuclear and electron motions may be decoupled (BORN and OPPENHEIMER, 1927, see also BORN and HUANG, 1954). This decoupling is equivalent to the assumption that the electrons see the nuclei as being fixed in position at any given moment, since they move much more rapidly than the nuclei due to their smaller masses.

It is easy to visualize the electronic charge distribution of the ion core moving with the nucleus as it vibrates. However, such behaviour is less evident for the valence electrons. Nevertheless, it turns out that something like that also occurs for the valence electrons.

According to the Born-Oppenheimer or adiabatic approximation in a solid there exists a many-body potential Φ governing the motions of the atoms. A calculation of Φ requires that we freeze the ions in each instantaneous configuration, and calculate the energy of the electrons. Φ is then, in essence, this energy plus the electrostatic energy of the ion-ion interaction. The phenomenological theory of lattice dynamics is based on the existence of Φ. But also the microscopic theory of lattice dynamics often uses the adiabatic approximation. Moreover, the adiabatic approximation is an important tool on describing the dynamical response of a lattice to external radiation (see appendix 3). It seems therefore reasonable to outline this approximation here.

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[1] Here we closely follow the standard monographs on lattice dynamics by BORN and HUANG (1954) and MARADUDIN et al. (1971) (see also, e. g., BRÜESCH, 1982).

To do this we start from the following total Hamiltonian for a crystal containing ions and (valence) electrons:

$$\mathscr{H} = T_{\mathrm{el}} + V_{\mathrm{el}} + T_{\mathrm{ion}} + V_{\mathrm{ion}} + H_{\mathrm{int}}. \tag{1.1.1}$$

Here T_{el} is the kinetic energy of the electrons, V_{el} is the Coulomb energy of the electrons, T_{ion} is the kinetic energy of the ions, V_{ion} is the interaction energy of the ions and H_{int} describes the interaction between the electrons and the ions.

From the Hamiltonian (1.1.1) we abstract an electronic part

$$H_{\mathrm{el}} = T_{\mathrm{el}} + V_{\mathrm{el}} + V_{\mathrm{ion}} + H_{\mathrm{int}} \tag{1.1.2}$$

depending parametrically through V_{ion} and H_{int} on the ionic coordinates $\boldsymbol{R}$. Now we expand the solution Ψ of the full Schrödinger equation

$$\mathscr{H}\Psi = \mathscr{E}\Psi \tag{1.1.3}$$

in terms of the solutions ψ of

$$H_{\mathrm{el}}\psi_n = E_n\psi_n. \tag{1.1.4}$$

That is, we seek a solution of (1.1.3) in the form

$$\Psi(\boldsymbol{r}, \boldsymbol{R}) = \sum_n \chi_n(\boldsymbol{R})\, \psi_n(\boldsymbol{r}, \boldsymbol{R}), \tag{1.1.5}$$

where $\boldsymbol{r}$ denotes the electronic coordinates. $\chi_n(\boldsymbol{R})$ is a function only of $\boldsymbol{R}$ and is to be determined.

Substituting (1.1.5) into (1.1.3), and using (1.1.4) and the orthonormality of the ψ's we obtain

$$(T_{\mathrm{ion}} + E_n)\,\chi_n + \sum_m C_{nm}\chi_m = \mathscr{E}\chi_n, \tag{1.1.6}$$

where

$$C_{nm} = A_{nm} + B_{nm} \tag{1.1.7}$$

with

$$\left.\begin{aligned} A_{nm} &= -\sum_l \frac{\hbar^2}{M_l} \int \mathrm{d}\boldsymbol{r} \left(\psi_n^*(\boldsymbol{r}, \boldsymbol{R}) \frac{\partial}{\partial \boldsymbol{R}_l} \psi_m(\boldsymbol{r}, \boldsymbol{R})\right) \frac{\partial}{\partial \boldsymbol{R}_l}, \\ B_{nm} &= -\sum_l \frac{\hbar^2}{2M_l} \int \mathrm{d}\boldsymbol{r} \left(\psi_n^*(\boldsymbol{r}, \boldsymbol{R}) \frac{\partial^2}{\partial \boldsymbol{R}_l^2} \psi_m(\boldsymbol{r}, \boldsymbol{R})\right), \end{aligned}\right\} \tag{1.1.8}$$

where M_l and $\boldsymbol{R}_l$ denote the mass and the position of the lth ion, respectively.

In absence of a magnetic field the ψ's can be chosen to be real, i.e. we have $A_{nn} = 0$, since the functions $\psi_n(\boldsymbol{r}, \boldsymbol{R})$ have been assumed to be normalized to unity for all $\boldsymbol{R}$.

When the terms involving nondiagonal elements of A and B (i.e. A_{nm} and B_{nm} for $n \neq m$) are dropped, the vibrational wave function is determined by the properties of the nth electronic state only, and no electronic transitions

accompany the ionic motion. In this case (1.1.6) becomes

$$(T_{\text{ion}} + E_n + C_n)\,\chi_{nv} = \mathcal{E}_{nv}\chi_{nv}, \tag{1.1.9}$$

where $C_n \equiv C_{nn} = B_{nn}$. In this equation v can be regarded as a vibrational quantum number. Adopting (1.1.9) the wave function of the combined system of electrons and ions reads for a state with energy $\mathcal{E}_{nv}$

$$\Psi_{nv}(\boldsymbol{r}, \boldsymbol{R}) = \chi_{nv}(\boldsymbol{R})\,\psi_n(\boldsymbol{r}, \boldsymbol{R}). \tag{1.1.10}$$

The first factor of the wave function (1.1.10) describes the ionic motion, and the second factor shows that during the ionic motion the electrons move as if the ions were fixed in their instantaneous positions. The electrons are said to follow adiabatically the motion of the ions. The approximation (1.1.10) for the total wave function is called adiabatic approximation.

To see what the adiabatic approximation implies we use the Born-Oppenheimer expansion in the following. We begin by writing

$$\boldsymbol{R}_l = \boldsymbol{R}_l^0 + \varkappa \boldsymbol{u}_l, \tag{1.1.11}$$

where $\boldsymbol{R}_l^0$ denotes the equilibrium position of the lth ion, $\boldsymbol{u}_l$ the displacement of the lth ion, and $\varkappa$ the expansion parameter. In the limiting case $M \to \infty$ (M denotes a characteristic mass of an ion) we must have $\varkappa \to 0$. Since $\varkappa$ is a dimensionless parameter, this suggests $\varkappa = (m/M)^\alpha$ with $\alpha > 0$, where m denotes the electronic mass.

To determine the exponent α, the Hamiltonian (1.1.2) is expanded formally in powers of the ionic displacements

$$H_{\text{el}}(\boldsymbol{r}, \boldsymbol{R}) = H_{\text{el}}(\boldsymbol{r}, \boldsymbol{R}^0 + \varkappa \boldsymbol{u}) = \sum_s \varkappa^s H_{\text{el}}^{(s)}(\boldsymbol{r}, \boldsymbol{R}^0), \tag{1.1.12}$$

where $H_{\text{el}}^{(s)}(\boldsymbol{r}, \boldsymbol{R}^0)$ is a homogeneous function of degree s in $\boldsymbol{u}$. We can fix α by noting that if $\alpha = 1/4$, $\varkappa^2 H_{\text{el}}^{(s)}$ is of the same order in $\varkappa$ as

$$T_{\text{ion}} = -\varkappa^{(1/\alpha)-2} \sum_l (M/M_l)\,(\hbar^2/2m)\,\nabla_{\boldsymbol{u}_l}^2 \equiv \varkappa^{(1/\alpha)-2} H_1(\boldsymbol{u}). \tag{1.1.13}$$

As will be shown below, to this order we have a harmonic Hamiltonian.

Expanding the wave function $\psi_n(\boldsymbol{r}, \boldsymbol{R}) = \psi_n(\boldsymbol{r}, \boldsymbol{R}^0 + \varkappa \boldsymbol{u})$ as a series in $\varkappa \boldsymbol{u}$, it can be readily seen from (1.1.8) that A_{nm} begins with a term $O(\varkappa^3)$, while B_{nm} begins with a term $O(\varkappa^4)$. Thus the operator C_n in (1.1.9) begins with a constant term $O(\varkappa^4)$.

In the adiabatic approximation the wave function (1.1.10) turns out to be exact to $O(\varkappa^2)$ and the energy $\mathcal{E}_{nv}$ to $O(\varkappa^5)$. To see this we expand χ_m in terms of the functions

$$\chi_m = \sum_v c_v^{(m)} \chi_{mv}. \tag{1.1.14}$$

When this expansion is substituted into (1.1.6) and use is made of (1.1.9) we obtain the following equation for $c_v^{(m)}$:

$$(\mathcal{E}_{mv} - \mathcal{E})\,c_v^{(m)} + \sum_{n(\neq m)} \sum_{v'} \langle mv|\, C_{mn}\, |nv'\rangle\, c_{v'}^{(n)} = 0. \tag{1.1.15}$$

On iterating (1.1.15) all the $c_{v'}^{(n)}$'s ($nv' \neq mv$) may be expressed by $c_v^{(m)}$. In this manner we obtain to the lowest order of approximation

$$\mathcal{E} = \mathcal{E}_{mv} + \sum_{n(\neq m)}{}' \sum_{v'} \langle mv| C_{mn} |nv'\rangle \langle nv'| C_{mn} |mv\rangle / (\mathcal{E}_{mv} - \mathcal{E}_{nv'}). \quad (1.1.16)$$

The second term on the right hand side of this equation describes the change of the energy due to C_{mn} ($n \neq m$), i.e. due to transitions between different electronic states. Since C_{mn} is at least of $O(\varkappa^3)$, this term begins with $O(\varkappa^6)$, i.e. $\mathcal{E}_{mv}$ is the exact energy to $O(\varkappa^5)$.

For a state with the energy (1.1.16) it holds $c_v^{(m)} \approx 1$ and for the elements $c_{v'}^{(n)}$ ($n \neq m$) we obtain from (1.1.15)

$$c_{v'}^{(n)} = \langle nv'| C_{nm} |mv\rangle / (\mathcal{E}_{mv} - \mathcal{E}_{nv'}). \quad (1.1.17)$$

Since C_{mn} is of $O(\varkappa^3)$, C_{mn} yields a contribution to χ_m of $O(\varkappa^3)$. Accordingly, χ_{mv} from (1.1.9) describes the ionic motion exact to $O(\varkappa^2)$.

Hence, in the Born-Oppenheimer expansion non-adiabatic terms appear only in a relatively high order in $\varkappa = (m/M)^{1/4}$. As $\varkappa$ never exceeds 1/10, the expansion may be expected to converge quickly.

As stated above, the expansion of C_n begins with a constant term of $O(\varkappa^4)$. It follows a term of $O(\varkappa^5)$ linear in $\boldsymbol{u}$. Thus, to $O(\varkappa^4)$ in the adiabatic approximation the ionic motion is governed solely by the electronic energy $E_n(\boldsymbol{R})$. An account of terms of $O(\varkappa^5)$ gives a contribution linear in $\boldsymbol{u}$ arising from C_n, but the motion remains adiabatic.

Now let us solve (1.1.9) by perturbation theory. To this end we expand E_n, χ_{nv}, and $\mathcal{E}_{nv}$ in a series using $\varkappa$ as small parameter. We use the same notation as in (1.1.12), i.e. an expansion coefficient of sth order is labelled by an upper index s. Note that $\mathcal{E}^{(s)}$ is a constant, while $E_n^{(s)}$ is a quantity of sth degree in $\boldsymbol{u}$. Comparing the expression resulting from (1.1.9) term by term we obtain

$$\mathcal{E}_{nv}^{(0)} = E_n^{(0)}(\boldsymbol{R}^0), \quad (1.1.18)$$

$$\mathcal{E}_{nv}^{(1)} = E_n^{(1)} = \sum_l \left(\partial E_n(\boldsymbol{R})/\partial \boldsymbol{R}_l\right)_{\boldsymbol{R}^0} \boldsymbol{u}_l = 0. \quad (1.1.19)$$

The identical vanishing of $E_n^{(1)}$ results from the fact that $\mathcal{E}_{nv}^{(1)}$ is independent of $\boldsymbol{u}$. From (1.1.19) follows that in the nth electronic state the equilibrium configuration $\boldsymbol{R}^0$ is defined by

$$\left(\partial E_n(\boldsymbol{R})/\partial \boldsymbol{R}_l\right)_{\boldsymbol{R}^0} = 0. \quad (1.1.20)$$

On account of (1.1.19) we obtain from the second order expression

$$[H_1 + E_n^{(2)} - \mathcal{E}_{nv}^{(2)}]\, \chi_{nv}^{(0)} = 0 \quad (1.1.21)$$

or

$$\left[T_{\text{ion}} + (\varkappa^2/2) \sum_{ll'} \boldsymbol{u}_l \left(\frac{\partial^2 E_n}{\partial \boldsymbol{R}_l\, \partial \boldsymbol{R}_{l'}}\right)_{\boldsymbol{R}^0} \boldsymbol{u}_{l'} - \varkappa^2 \mathcal{E}_{nv}^{(2)}\right] \chi_{nv}^{(0)} = 0. \quad (1.1.22)$$

(1.1.22) obviously describes harmonic vibrations of the ions about their equilibrium positions. The corresponding approximation is called the harmonic approximation. To this approximation the wave function of the crystal reads

$$\Psi_{n\nu}(\boldsymbol{r}, \boldsymbol{u}) = \chi_{n\nu}^{(0)}(\boldsymbol{u})\, \psi_n^{(0)}(\boldsymbol{r}, \boldsymbol{R}^0) \tag{1.1.23}$$

and the corresponding eigenvalue is given by

$$\mathscr{E}_{n\nu} = E_n^{(0)}(\boldsymbol{R}_0) + \varkappa^2 \mathscr{E}_{n\nu}^{(2)}. \tag{1.1.24}$$

The latter two equations have been obtained by substituting (1.1.10) into (1.1.3), accounting for (1.1.4), and expanding the quantities with respect to $\varkappa$. We see that the harmonic approximation is a special case of the adiabatic approximation. When we continue the expansion procedure beyond the second order, anharmonic terms occur in (1.1.9).

Concluding this section, let us briefly discuss the validity of the adiabatic approximation. A corresponding criterion may be obtained from (1.1.17) by requiring that $|c_\nu^{(n)}| \ll 1$ for $n \neq m$. Using (1.1.8), the virial theorem, and the fact that in a solid the mean square amplitude of an atom is proportional to ω^{-1} (ω — characteristic vibrational frequency; cf. (1.4.51)), we obtain the criterion $\hbar\omega/|\mathscr{E}_{m\nu} - \mathscr{E}_{n\nu'}| \ll 1$. This criterion is quite well satisfied in the case of insulators and semiconductors due to the large gaps in the electronic spectra. Non-adiabatic effects have been found in narrow gap semiconductors (Sherrington, 1971). The above criterion is violated in metals. Nevertheless, it turns out that in metals in general the adiabatic approximation is valid (see Brovman and Kagan, 1974). Non-adiabaticity is governed in metals by the parameter $\hbar\omega/\varepsilon_F$ (ε_F — Fermi energy). Note that there is some indication that non-adiabaticity may occur in materials with strong electron correlation (cf. Kondo and Yamadji, 1977).

1.2. Force constants and their properties

In the preceding section we found that the motion of the atoms in a solid may be described in general by a many-body potential depending on the instantaneous atomic positions.

On dissociating the instantaneous position $\boldsymbol{R}(l)$ of the lth atom into a rest position $\boldsymbol{x}(l)$ and a displacement $\boldsymbol{u}(l)$ according to

$$\boldsymbol{R}(l) = \boldsymbol{x}(l) + \boldsymbol{u}(l) \tag{1.2.1}$$

we can formally expand Φ in powers of the displacements:

$$\Phi = \Phi_0 + \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{\substack{\alpha_1 \ldots \alpha_n \\ l_1 \ldots l_n}} \Phi_{\alpha_1 \ldots \alpha_n}(l_1 \ldots l_n)\, u_{\alpha_1}(l_1) \ldots u_{\alpha_n}(l_n). \tag{1.2.2}$$

Here $u_\alpha(l)$ is the αth cartesian component of $\boldsymbol{u}(l)$, Φ_0 the potential energy of the static lattice and

$$\Phi_{\alpha_1 \ldots \alpha_n}(l_1 \ldots l_n) = \left. \frac{\partial^n \Phi}{\partial u_{\alpha_1}(l_1) \ldots \partial u_{\alpha_n}(l_n)} \right|_0, \tag{1.2.3}$$

where the subscript 0 means that the derivatives are evaluated with all the atoms in their rest positions.

From (1.2.3) it follows that the coefficients $\Phi_{\alpha_1 \dots \alpha_n}(l_1 \dots l_n)$ are completely symmetric in the indices $l_1\alpha_1, l_2\alpha_2, \dots$.

On considering the force acting on the lth atom in α-direction

$$F_\alpha(l) = -\partial\Phi/\partial u_\alpha(l)$$

$$= -\Phi_\alpha(l) - \sum_{n=1}^{\infty} \sum_{\substack{\alpha_1 \dots \alpha_n \\ l_1 \dots l_n}} \frac{1}{n!} \Phi_{\alpha\alpha_1 \dots \alpha_n}(l l_1 \dots l_n)\, u_{\alpha_1}(l_1) \dots u_{\alpha_n}(l_n) \quad (1.2.4)$$

the physical meaning of the coefficients $\Phi_{\alpha_1 \dots \alpha_n}(l_1 \dots l_n)$ becomes evident: $-\Phi_\alpha(l)$ is the force in α-direction acting on the lth atom when it and the other atoms in the crystal are in their rest positions, $-\Phi_{\alpha\alpha_1}(l l_1)$ is, to the first order of accuracy, the α-component of the force on the lth atom due to a unit displacement of the l_1th atom in α_1-direction, etc. Consequently, the coefficients $\Phi_\alpha(l)$, $\Phi_{\alpha\alpha_1}(l l_1)$, $\Phi_{\alpha\alpha_1\alpha_2}(l l_1 l_2), \dots$ are called atomic force constants of the first, second, third, ... order, respectively.

If the rest positions of the atoms are also equilibrium positions, the first order force constant $\Phi_\alpha(l)$ vanishes identically. While in a finite crystal the absence of a net force acting on any atom, i.e. $\Phi_\alpha(l) = 0$, is the only condition for a coincidence of the rest and equilibrium positions, in an infinite crystal the equilibrium condition is two-fold (BORN and HUANG, 1954, section 23; see also SARKAR and SENGUPTA, 1977): (i) $\Phi_\alpha(l) = 0$ for any atom, (ii) the configuration corresponds to vanishing stresses. In a finite crystal the latter condition is automatically fulfilled, if the former one is satisfied (for any atom including those near the surface).

For the study of certain problems, e.g. of effects caused by external stresses or strains on dynamical properties of a crystal, it is convenient to expand the lattice potential around rest positions which differ from equilibrium positions (see also section 4.2.).

Apart from specific features characterizing a special lattice, the force constants $\Phi_{\alpha_1 \dots \alpha_n}(l_1 \dots l_n)$ are subjected to a number of general restrictions resulting from certain invariance conditions every solid must obey. There are two types of such restrictions. The first type follows from the invariance of the lattice potential and its derivatives with respect to the atomic displacements, when the lattice is subjected to infinitesimal rigid displacements (translations, rotations). The second type is connected with the symmetry and structure of a particular crystal.

If the lattice as a whole is subjected to an infinitesimal rigid body displacement $\boldsymbol{r}$ the lattice potential and its derivatives must remain unchanged. On replacing in (1.2.2) $\boldsymbol{u}$ by $\boldsymbol{r}$ this condition yields

$$\sum_{\substack{\alpha_1 \dots \alpha_n \\ l_1 \dots l_n}} \Phi_{\alpha_1 \dots \alpha_n}(l_1 \dots l_n)\, v_{\alpha_1} \dots v_{\alpha_n} = 0 \qquad (n = 1, 2, \dots), \quad (1.2.5)$$

where v_α is the α-component of $\boldsymbol{v}$. Since (1.2.5) must hold for all values of $\boldsymbol{v}$,