

Field theoretical approach to fluxes in crystals(*)

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THE DYNAMICS of a crystal lattice with an internal two-particle interaction is described as a limiting case of a continuous dynamical system with a nonlocal internal interaction. For this kind of dynamics a variational principle is formulated in terms of a Lagrangian density in substantial coordinates. These substantial coordinates are similar to the usual Lagrangian coordinates in hydrodynamics. As in hydrodynamics, a conversion from substantial into local or Eulerian coordinates can be made. In fact, this conversion is an inversion of the function that describes the position of the material points as a function of the substantial coordinates. Within the Lagrangian, the conversion from substantial into local coordinates is carried out to obtain a Lagrangian in terms of local coordinates. With both Lagrangians, conservation laws for the linear momentum and for the energy are derived. This is done with a version of Noether's theorem which differs slightly from the usual one. In this way explicit expressions are found for the currents of linear momentum and energy in crystals through points fixed in the material as well as through points fixed in the laboratory. Additionally, in both coordinate systems the balance equation for a quantity which may be identified as the quasi-momentum is constructed.

Opisano dynamikę siatki krystalicznej z dwucząsteczkowym oddziaływaniem wewnętrznym, jako graniczny przypadek dynamicznego układu ciągłego z nielokalnym oddziaływaniem wewnętrznym. Sformułowano zasadę wariacyjną, wyrażoną przez gęstość Lagrangianu we współrzędnych materialnych. Współrzędne te są podobne do zwykłych współrzędnych Lagrange'a w hydrodynamice. Tak jak i w hydrodynamice można tu dokonać przejścia od współrzędnych materialnych do współrzędnych lokalnych (lub Eulera). Przejście to jest odwróceniem funkcji opisującej położenie punktów materialnych. Aby wyrazić Lagrangian przez lokalne współrzędne, dokonano przejścia od współrzędnych materialnych do współrzędnych lokalnych. Wykorzystując oba Lagrangiany wyprowadzono prawa zachowania pędu i energii. Posłużono się w tym celu nieco zmodyfikowanymi twierdzeniami Noethera. Znalezione w ten sposób strumienie pędu i energii przechodzące przez punkty kryształu ustalone w materiale oraz w laboratorium. Ponadto skonstruowano w obu układach współrzędnych równania równowagi dla pewnej wielkości, która jest określona jako quasi-pęd.

Динамика кристаллической решетки с внутренними бинарными взаимодействиями описывается в качестве предельного случая континуальной динамической системы с нелокальными внутренними взаимодействиями. Вариационный принцип для такого рода динамики формулируется через плотность функции Лагранжа в материальных координатах. Проводится преобразование выражения для функции Лагранжа с целью выражения ее через локальные координаты. Оба представления функции Лагранжа используются для вывода законов сохранения импульса и энергии. Используется видоизменная по сравнению с обычной теорема Нетер. Этим путем были найдены явные выражения для потоков импульса и энергии в кристаллах как для фиксированной материальной точки, так и для фиксированной точки в лабораторной системе отчета. Добавочно в обеих координатных системах получено уравнение баланса для величины, которую можно отождествлять с квази-импульсом.

1. Introduction

IN THE LITERATURE on solid state physics, a lot of rather unclear and apparently contradictory remarks have been made about the densities and fluxes of energy, linear momentum

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and quasi-momentum in crystals. Nevertheless, the knowledge of the explicit expressions for the densities and fluxes of energy and linear momentum are of great importance for the calculation of transport coefficients such as the coefficients for heat conduction and viscosity.

In order to try to keep the analogy with photons as close as possible in solid state physics one usually works already from the beginning with phonon variables. This method does not elucidate much because besides the many analogies between the theory of crystal vibrations on the one hand and the electro-magnetic theory on the other hand, there are also essential differences:

(i) The theory of the electromagnetic field is a covariant theory; consequently, the energy flux and linear momentum density are proportional to each other.

(ii) In most descriptions of crystal vibrations, waves with an infinite wavelength ($k = 0$) may appear. For the electromagnetic field such waves do not have any meaning.

In the field theory, the current of some conserved quantity as energy and linear momentum is defined as the flux term of the local conservation law for this conserved quantity.

For example, if the equation of motion yields⁽¹⁾

$$(1.1) \quad d/dt E + d/dx S \doteq 0,$$

and E is the energy density, then S is the energy flux or energy current. If the equation of motion is derivable from a variational principle (Hamilton's principle or action principle), relations of the form (1.1) can be derived systematically with Noether's theorem.

2. Substantial coordinates

Let us consider a continuous dynamical system. (For simplicity, we assume here the system to be one-dimensional). Let the state of the system be defined by the field $u(m)$ and the field velocity $\dot{u}(m)$ as a function of the coordinate m . The coordinate m itself will be interpreted as a substantial coordinate, indicating material points of the system. For example, one can take the position at $t = 0$ or at equilibrium as the corresponding substantial coordinate. The coordinate m labels material points of the medium analogous to particle indices in usual lattice dynamics and Lagrangian coordinates in hydrodynamics.

The system dynamics is described by a function $u(m, t)$. This function gives the time evolution of the field $u(m)$. The field velocity then is $\dot{u} = (d/dt u)_m$. We assume that the equations of motion can be derived from a Lagrange functional. This functional must be taken such that the equations of motion describe the crystal lattice dynamics as a limiting case. Therefore, we assume the dynamical system to be inhomogeneous and to have a non-local internal interaction. Then, a reasonable "ansatz" for a Lagrangian is

$$(2.1) \quad \mathcal{L} = \int L(m) dm,$$

$$(2.2) \quad L(m) = \frac{1}{2} \rho_0(m) \dot{u}^2(m) - \int d\mu V(z(m, \mu), m, \mu),$$

$$(2.3) \quad z(m, \mu) = \mu + u(m + \mu) - u(m).$$

(1) The weak identity \doteq is used to indicate that the equality only holds for solutions u of the equation of motion.

The two terms in Eq. (2.2) are the kinetic and the potential energy density, respectively. Both densities are densities in m -space. The function $V(z, m, \mu)$ describes the interaction between the material points m and $(m + \mu)$ of distance $z(m, \mu)$. The function $\rho_0(m)$ is the substantial mass density.

From Eq. (2.2) one obtains in the usual way the equation of motion

$$(2.4) \quad \rho_0(m)\ddot{u}(m) \doteq \int d\mu [V'(z(m, \mu), m, \mu) - V'(z(m - \mu, \mu), m - \mu, \mu)],$$

where

$$(2.5) \quad V'(z, m, \mu) = d/dz V(z, m, \mu).$$

With a suitable choice for $\rho_0(m)$ and for $V(z, m, \mu)$, Eq. (2.4) yields the equation of motion for an arbitrary crystal lattice with an internal two-particle interaction.

3. Local conservation laws

Usually, one applies Noether's theorem to systems with a local internal interaction only [1, 2]. The use of the formula

$$(3.1) \quad F(m) - F(m - \mu) = d/dm \int_{-\mu}^0 F(m + \eta) d\eta$$

allows us to extend the method to systems with a nonlocal internal interaction. Thus Noether's theorem can be applied to Lagrangians of the form (2.2).

From Eqs. (3.1) and (2.1) one deduces directly the "strong" identity

$$(3.2) \quad \delta L = - \left\{ \rho_0(m)\ddot{u}(m) - \int d\mu [V'(z(m, \mu), m, \mu) - V'(z(m - \mu, \mu), m - \mu, \mu)] \right\} \delta u \\ + d/dt(\rho_0(m)\dot{u}(m)\delta u) - d/dm \int_{-\mu}^0 d\eta V'(z(m + \eta, \mu), m + \eta, \mu) \delta u(m + \mu + n).$$

Using the equation of motion (2.4), Eq. (3.2) becomes the "weak" identity

$$(3.3) \quad \delta L \doteq d/dt(\rho_0(m)\dot{u}(m)\delta u) + d/dm \int_{-\mu}^0 d\eta V'(z(m + \eta, \mu), m + \eta, \mu) \delta u(m + \mu + n).$$

On the other hand, a strong identity for δL can be derived directly with Eq. (2.1) and an explicit expression for δu . If one takes for instance $\delta u = \varepsilon$, then

$$(3.4) \quad \delta L = 0$$

and one has the local conservation law

$$(3.5) \quad d/dt(\rho_0(m)\dot{u}) - d/dm \int_{-\mu}^0 d\eta V'(z(m + \eta, \mu), m + \eta, \mu) \doteq 0.$$

More generally one can state the following: For any variation δu that leaves the Lagrangian density L invariant up to a total derivative (Noetherian variation), a local conservation law of the form (1.1) can be derived. One can show [1] that this formulation is equivalent to Noether's theorem.

Obviously, the quantity $\varrho_0(m)\dot{u}$ is the linear momentum density in m -space. Then $-\int d\mu \int_{-\mu}^0 d\eta V'(z(m+\eta, \mu), m+\eta, \mu)$ is the substantial linear momentum flux, i.e. the linear momentum current through a point m fixed in the material (material point), and Eq. (3.5) is the local conservation law for the linear momentum. Analogously, the variation $\delta t = \varepsilon$ leaves the action $\int \mathcal{L} dt$ invariant, or the variation $\delta u = \varepsilon \dot{u}$ leaves L invariant up to a term $\varepsilon d/dt L$. This yields the local conservation law

$$(3.6) \quad d/dt \left[\frac{1}{2} \varrho_0(m) \dot{u}^2 + \int d\mu V(z, m, \mu) \right] - d/dm \int d\mu \int_{-\mu}^0 d\eta V'(z(m+\eta, \mu), m+\eta, \mu) \dot{u}(m+\mu+\eta) \doteq 0$$

which is clearly the local conservation law for the energy. The quantity

$$-\int d\mu \int_{-\mu}^0 d\eta V'(z(m+\eta, \mu), m+\eta, \mu) \dot{u}(m+\mu+\eta)$$

is the substantial energy flux.

4. A local balance equation

For homogeneous media, i.e.

$$(4.1) \quad V(z, m, \mu) = \bar{V}(z, \mu), \quad \varrho_0(m) = \bar{\varrho},$$

there is another Noetherian variation, namely $\delta m = \varepsilon$ or equivalently $\delta u = \varepsilon du/dm = \varepsilon u'$. The corresponding local conservation law is

$$(4.2) \quad d/dt [-\bar{\varrho} \dot{u} u'] + d/dm \left[\frac{1}{2} \bar{\varrho} \dot{u}^2 - \int d\mu \bar{V}(z, \mu) + \int d\mu \int_{-\mu}^0 d\eta \bar{V}'(z(m+\eta, \mu), \mu) u'(m+\mu+\eta) \right] \doteq 0.$$

Without further explanation in the literature, equations equivalent to Eq. (4.2) are sometimes called the conservation law for momentum [3]. However, this terming is misleading because of the following reason: The only argument for the terming lies in the analogy with the electro-magnetic (e.m.) theory, but there are also many essential differences. For example, the e.m. theory is a Lorentz-invariant theory and the theory of condensed matter is usually treated non-relativistically. Therefore, in the e.m. theory (linear) momentum density and energy flux are proportional, whereas in condensed matter these quantities are physically not related. We obtain a more precise terming by calling Eq. (4.2) the local conservation law for the "quasi-momentum". Then, with suitable phonon variables, the "total quasi-momentum" $-\int \bar{\varrho} \dot{u} u' dm$ can be written as $\sum k N_k$, N_k being the classical analogue of the number operator of phonons with the wave number k . In the e.m. theory, the total linear momentum as well as the energy flux can be written in this form. In the general inhomogeneous case, neither the variation $\delta u = \varepsilon u'$ nor $\delta m = \varepsilon$ are Noetherian

variations. Then, the same methods which have lead to Eq. (4.2) lead to the local balance equation

$$(4.3) \quad d/dt[-\rho_0(m)\dot{u}u'] + d/dm \left[\frac{1}{2} \rho_0(m)\dot{u}^2 - \int d\mu V(z(m, \mu), m, \mu) + \int d\mu \int_{-\mu}^0 d\eta V'(z(m+\eta, \mu), m+\eta, \mu) u'(m+\mu+\eta) \right] \\ \doteq \frac{1}{2} \rho'(m)\dot{u}^2 - \int d\mu V_m(z(m, \mu), m, \mu),$$

where

$$(4.4) \quad V_m(z, m, \mu) = d/dm V(z, m, \mu).$$

In analogy to the relation (4.2), Eq. (4.3) is interpreted as the local balance equation for the "quasi-momentum".

For the application to crystal lattices, we note that for lattices the derivatives u' are not defined. Thus, strictly speaking, Eq. (4.3) cannot be applied to crystal lattices. Nevertheless, in the literature on crystals the quasi-momentum k of a phonon is a familiar concept. Therefore, it is worthwhile to study whether it is possible to define u' in a discrete lattice such that Eq.(4.3) makes sense.

With periodic boundary conditions a usual decomposition of u in Bloch functions is (again we assume a mono-atomic lattice)

$$u(la) = \sum_{k \in \mathcal{B}} w(k) \exp i k l a,$$

where

$$\mathcal{B} = \{k | k = 2\pi n/L, n \in \mathcal{Z}, -N/2 < n \leq N/2\},$$

and N is the number of lattice points, a the interatomic distance, $L = Na$ and \mathcal{Z} is the set of all integers.

The restriction of k to the first Brioullin zone \mathcal{B} is arbitrary. We can drop this restriction, but then $w(k)$ is not defined uniquely anymore. We obtain a continuum representation $u(m)$ of $u(la)$ for example by taking

$$u(la) \rightarrow u(m) = \sum_{k \in \mathcal{B}} w(k) \exp i k m.$$

For such a continuum representation the total quasi-momentum $\int i u' dm$ reads $\sum k N_k$ and the total production $\int Q dm = 0$. Thus, globally the quasi-momentum is conserved, but its definition is not unique.

If the dynamics of the crystal with its continuum representation is developed without the restriction $k \in \mathcal{B}$, $w(k)$ will, in general, not vanish for $k \notin \mathcal{B}$.

A restriction of $k \in \mathcal{B}$,

$$w(k) \rightarrow w'(k) = 0 \quad (k \notin \mathcal{B})$$

$$w'(k) = \sum_{K \in \mathcal{K}} w(k+K), \quad (k \in \mathcal{B}),$$

\mathcal{K} being the reciprocal lattice of the crystal, does not change the values of u at the lattice points, but it does for the derivatives u' and, consequently, for the total quasi-momentum. The consequence is that quasi-momentum changes in the same way as by, what is called, Umklapp processes.

5. Local coordinates

Only a minority of papers in the field of solid state physics concerning fluxes in crystals deal with fluxes corresponding to the use of substantial coordinates [4]. In most papers fluxes corresponding to the use of local coordinates are discussed [5–8]. In the present formalism conversion of the results for a substantial coordinate frame into a local coordinate frame can be performed. Let us discuss this conversion.

The position of a material point is given by

$$(5.1) \quad x = q(m) = m + u(m).$$

Now we introduce the inverse function $\tilde{q}(x)$ and put

$$(5.2) \quad m = \tilde{q}(x) = x + v(x),$$

where

$$(5.3) \quad x = q(\tilde{q}(x)), \quad m = \tilde{q}(q(m)).$$

Then one sees easily that

$$(5.4) \quad v(x) + u(x + v(x)) = 0, \quad u(m) + v(m + u(m)) = 0.$$

Analogously to the discussion for fluid motion in [9], the Lagrangians (2.1) and (2.2) can be converted with Eq. (5.4) into a Lagrangian which describes the system in terms of $v(x)$:

$$(5.5) \quad \mathcal{L} = \int \bar{L} dx,$$

$$(5.6) \quad \bar{L} = \frac{1}{2} \rho(x) \dot{u}^2(x) - J(x) \int dz J(x+z) V(z, x+v, z+v(x+z)-v),$$

where

$$(5.7) \quad \dot{u}(x) = - \frac{\dot{v}(x)}{1+v'(x)},$$

$J(x)$ is the Jacobian of the transformation $m \rightarrow x$

$$(5.8) \quad J(x) = \det(\partial m / \partial x) = 1 + v',$$

and

$$(5.9) \quad \rho(x) = J(x) \rho_0(x + v(x))$$

is the usual (hydrodynamical) local mass density as a function of the local (Eulerian) coordinate x . In Eqs. (5.5) and (5.6) only $v(x)$ can be varied independently. For all other variations, as for instance $\rho(x)$ and $J(x)$, the formulae (5.4) have to be used.

Now we are prepared for the discussion of the conservation laws and the balance equation in local coordinates.

The Noetherian variation $\delta u = \varepsilon$ for the system (2.1) is equivalent to the variation $\delta v = -\varepsilon(1+v')$ which is a Noetherian variation for Eq. (5.6). The corresponding local conservation law is

$$(5.10) \quad \partial/\partial t[\rho(x)\dot{u}] + d/dx \left[\rho(x)\dot{u}^2 - \int_{-\mu}^0 d\eta V'(z(x+v+\eta), x+v+\eta, \mu) \right] \doteq 0,$$

where $\partial/\partial t$ means differentiation with respect to t at constant x . Clearly, $\rho(x)\dot{u}$ is the local linear momentum density. The flux that appears in Eq. (5.10) is the local linear momentum flux, i.e. the current of the linear momentum through a point fixed in the laboratory frame. Analogously, we find with $\delta t = \varepsilon$ or, equivalently, with $\delta u = \varepsilon\dot{u}$ or $\delta v = \varepsilon\dot{v}$, the local conservation law for the energy in the local coordinate frame:

$$(5.11) \quad \partial/\partial t \left[\frac{1}{2} \rho(x)\dot{u}^2 + J(x) \int d\mu V(z(x+v, \mu), x+v, \mu) \right] \\ + d/dx \left[\frac{1}{2} \rho_0(x)\dot{u}^3 + J(x)\dot{u} \int d\mu V(z(x+v, \mu), x+v, \mu) \right. \\ \left. - \int_{-\mu}^0 d\eta \dot{u}(x+v+\eta+\mu) V'(z(x+v+\eta, \mu), x+v+\eta, \mu) \right] \doteq 0.$$

The local balance equation for the quasi-momentum in the local coordinate frame is obtained by means of the variation $\delta m = \varepsilon$ or, equivalently, $\delta u = \varepsilon u'$ or $\delta v = \varepsilon v'$:

$$(5.12) \quad \partial/\partial t [-\rho(x)\dot{u}u'] + d/dx \left[-\frac{1}{2} \rho(x)\dot{u}^2 u' + \frac{1}{2} \rho(x)\dot{u}^2 - \int d\mu V(z(x+v, \mu), x+v, \mu) \right. \\ \left. + \int_{-\mu}^0 d\eta u'(x+v+\eta+\mu) V'(z(x+v+\eta, \mu), x+v+\eta, \mu) \right] \\ \doteq \rho'_0(x+v) J(x)\dot{u}^2 - J(x) \int d\mu V_m(z(x+v, \mu), x+v, \mu).$$

The formulae given above may be generalized easily to three dimensions [10] and applied to non-Bravais lattices [11]. Comparing these results with the literature [4-8], we obtain the connection between several different more intuitive approaches to the calculation of fluxes in crystals.

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