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Quasi-periodic Green's functions of the Helmholtz and Laplace equations

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Abstract

A classical problem of free-space Green's function $G_{0\Lambda}$ representations of the Helmholtz equation is studied in various quasi-periodic cases, i.e., when an underlying periodicity is imposed in less dimensions than is the dimension of an embedding space. Exponentially convergent series for the free-space quasi-periodic $G_{0\Lambda}$ and for the expansion coefficients D_L of $G_{0\Lambda}$ in the basis of regular (cylindrical in two dimensions and spherical in three dimension (3D)) waves, or lattice sums, are reviewed and new results for the case of a one-dimensional (1D) periodicity in 3D are derived. From a mathematical point of view, a derivation of exponentially convergent representations for Schlömilch series of cylindrical and spherical Hankel functions of any integer order is accomplished. Exponentially convergent series for $G_{0\Lambda}$ and lattice sums D_L hold for any value of the Bloch momentum and allow $G_{0\Lambda}$ to be efficiently evaluated also in the periodicity plane. The quasi-periodic Green's functions of the Laplace equation are obtained from the corresponding representations of $G_{0\Lambda}$ of the Helmholtz equation by taking the limit of the wave vector magnitude going to zero. The derivation of relevant results in the case of a 1D periodicity in 3D highlights the common part which is universally applicable to any of remaining quasi-periodic cases. The results obtained can be useful for the numerical solution of boundary integral equations for potential flows in fluid mechanics, remote sensing of periodic surfaces, periodic gratings, and infinite arrays of resonators coupled to a waveguide, in many contexts of simulating systems of charged particles, in molecular dynamics, for the description of quasi-periodic arrays of point interactions in quantum mechanics, and in various *ab initio* first-principle multiple-scattering theories for the analysis of diffraction of classical and quantum waves.

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1. Introduction

Let Λ be a d_Λ-dimensional simple (Bravais) periodic lattice embedded in a space of dimension $d \geqslant d_\Lambda$ (the condition of a simple lattice can easily be relaxed to an arbitrary periodic lattice by following recipes of [1–5]). Let $\mathcal{H}_l^+$ stand for the cylindrical $\left(H_l^{(1)}\right)$ and spherical $\left(h_l^{(1)}\right)$ Hankel functions in $d = 2$ and $d = 3$, respectively, $\mathcal{Y}_L$ be corresponding angular momentum harmonics (cylindrical in $d = 2$ and spherical in $d = 3$, see also appendix B for properties of $\mathcal{Y}_L$), and $\mathbf{r}$ and $\mathbf{r}'$ be spatial points. The paper is concerned with an efficient calculation of the series

$$\sum_{\mathbf{r}_n \in \Lambda} \mathcal{H}_l^+(\sigma|\mathbf{r} - \mathbf{r}' + \mathbf{r}_n|)\mathcal{Y}_L^*(\hat{\mathbf{r}}_n)\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_n}, \tag{1}$$

where the origin of coordinates is in the lattice, $\mathbf{k}$ is called the Bloch momentum, $\sigma = 2\pi/\lambda$ denotes a wave vector magnitude (σ is not necessarily equal to $|\mathbf{k}|$), λ is a wavelength, L is, in general, a multi-index of angular momentum numbers (e.g., $L = (lm)$ in three dimensions with $l \geqslant 0$ and $-l \leqslant m \leqslant l$), * stands for a complex conjugate, and $\hat{\mathbf{r}}_n$ denotes a unit vector which points in the direction of $\mathbf{r}_n$.

In mathematical literature such series are known as Schlömilch series [6–8]. As first noted by Emersleben [9], in three dimensions (3D) in the special case of $\mathbf{r} - \mathbf{r}' = 0$ and $l = \sigma = 0$ the series reduce to *Epstein zeta functions* [10–12]. A physical motivation to investigate such series derives from a fact that, for $l = 0$, the series (1) are prerequisite to determine a corresponding free-space (quasi-) periodic Green's function $G_{0\Lambda}$ of a scalar Helmholtz equation (see below). For $l \neq 0$ and $\mathbf{r} - \mathbf{r}' = 0$, with singular term being excluded, the series (1) then formally determine the lattice sums D_L, which are defined as the expansion coefficients $G_{0\Lambda}$ in the basis of cylindrical and spherical Bessel functions in 2D and 3D, respectively (see equations (8), (11)).

However, analytic closed expressions for such series are only known for $l = 0$ in two particular cases in 3D: (i) in the case of a one-dimensional (1D) periodicity [13–15] and, when additionally $\sigma = 0$ (the Laplace limit), (ii) for a two-dimensional (2D) periodicity [14]. Otherwise the summation in (1) has to be performed numerically. However, since

$$\mathcal{H}_l^+(z) \sim c_h z^{-(d-1)/2} \left(\frac{2}{\pi}\right)^{(d-1)/2} \exp\{\mathrm{i}[z - (d-1)\pi/4 - l\pi/2]\} \tag{2}$$

as $z \to \infty$ and $-\pi < \arg z < 2\pi$, where $c_h = 1$ unless $d = 2$, in which case $c_h = \sqrt{2/\pi}$ (see equations (9.2.3) and (10.1.1) of [16]), the series (1) is not absolutely convergent. Even if one assumes that σ has an infinitesimally small positive imaginary part, and thereby establishing absolute convergence, the convergence of the series in equation (1) is notoriously slow, thereby rendering it useless for practical applications.

The study of efficient techniques for the calculation of $G_{0\Lambda}$ and lattice sums D_L has a long history [1, 2, 4, 8, 17–24] and the topic has roots and branches in different areas of chemistry, physics and mathematics. Despite that it still continues to be a perennial research subject [5, 25–37]. However, quite often this happens merely because researches in widely differing areas of chemistry, physics and mathematics are not aware of the techniques and results developed in connection with the so-called Korringa–Kohn–Rostoker (KKR) [1, 2, 23, 24] and layer Korringa–Kohn–Rostoker (LKKR) theories either for quantum (electron) waves within low-energy electron diffraction (LEED) theory [4, 20–22] or for various classical (acoustic, elastic, electromagnetic, water) waves [5, 26, 27]. Therein *exponentially convergent* series for $G_{0\Lambda}$ and lattice sums D_L have been derived for a number of cases. In a *periodic case* ($d_\Lambda = d$), efficient computational schemes for $G_{0\Lambda}$ and lattice sums D_L have been provided more than 30 years ago [2, 23]. The quasi-periodic case $d_\Lambda = 2$ and $d = 3$ has been investigated in detail in a series of articles by Kambe almost 40 years ago [4, 20, 21]. The case $d_\Lambda = 1$ and $d = 2$ has been dealt with only relatively recently in [5, 26]. Surprisingly enough, the case $d_\Lambda = 1$ and $d = 3$ has not been studied in full detail yet, although it may provide an efficient description of 'wave-integrated circuits'.

Therefore, in the following we shall focus on the so-called *quasi-periodic*, or layer, case, when the underlying lattice Λ is of lower dimensionality than the embedding space ($d_\Lambda < d$) and, in particular, on the $d_\Lambda = 1, d = 3$ case. There are many physical problem which would profit from an efficient computational scheme for $G_{0\Lambda}$ and lattice sums D_L in the case of 1D periodicity in 3D. For instance, a Green's function representing a point source and satisfying the respective von Neumann and Dirichlet boundary condition on a flow channel walls in fluid mechanics for the flow between parallel planes can be written as a sum and difference of $G_{0\Lambda}$ corresponding to 1D periodicity in 3D taken at two different spatial points [30]. (For the flow in a rectangular channel, the relevant $G_{0\Lambda}$ would then correspond to 2D periodicity in 3D [30].) Another problem involves infinite arrays of resonators coupled to a waveguide which by itself may have a plethora of photonics applications [38]. Moreover, recent progress in nanotechnology made it possible to fabricate 1D chains of metal nanoparticles [39, 40] and dielectric microparticles [41]. Additionally, understanding of linear periodic arrays of lossless spheres is germane for the qualitative description of finite-length periodic arrays of small antennas [42]. In a linear chain of spherical metal nanoparticles light can be transmitted by electrodynamic interparticle coupling resulting in a subwavelength-sized light guide [39, 40, 43–45]. So far, infinite 1D linear chains of particles have only been investigated within the one-particle theory framework of Schrödinger equation for the description of polymers [15], in the electrostatic limit within the framework of the Laplace equation [44], or in the dipole approximation [42, 45, 46]. Moreover, the energy operator in the one-particle theory of periodic point (zero-range) interactions is constructed in terms of an auxiliary operator which corresponds essentially to the operator of multiplication by D_{00} (γ function of Karpeshina [13, 47]).

In the following, exponentially convergent series for the free-space quasi-periodic $G_{0\Lambda}$ and for the lattice sums D_L are reviewed and new results for the case of a 1D periodicity in 3D are derived (see equations (83), (102) and (118)). The derivation of relevant results for the case of a 1D periodicity in 3D is performed in such a way that the common part which is universally applicable to any of the remaining quasi-periodic cases is highlighted. Thereby, a link with earlier results by Kambe [4, 20] for a 2D periodicity in 3D can easily be established and the proof of results for a 1D periodicity in 2D announced in [26] can easily be carried out.

1.1. The outline of the paper

The paper is organized as follows. Section 2 introduces notation, provides some necessary definitions and gives an overview of some of the problems requiring the knowledge $G_{0\Lambda}$ and lattice sums. In section 3, $G_{0\Lambda}$ is expressed as an exponentially convergent sum over a dual lattice Λ^*. Such a dual representation of $G_{0\Lambda}$ is then a starting point in the derivation of a corresponding exponentially convergent Ewald representation of $G_{0\Lambda}$ in section 4. As in the bulk case, a derivation of the Ewald representation invokes a suitable integral representation of Hankel functions and a Jacobi identity (see appendix D). In addition, following Kambe [21], an analytic continuation procedure is employed, which is analogous to finding the values of the Riemann ζ-function outside the domain of absolute convergence of a defining series (see [48], p 273). The Ewald representation of $G_{0\Lambda}$, which is a hybrid sum over both Λ and dual lattice Λ^*, converges uniformly and absolutely over bounded sets of $\mathbf{R}$. Unlike the dual representation, the Ewald representation can also be efficiently evaluated in the periodicity plane (provided that it remains $\mathbf{R} \notin \Lambda$).

Exponentially convergent series for the lattice sums D_L in the case of a 1D periodicity in 3D are derived in section 5. Equations (83), (102), (118) are the main new results of this paper.

In section 6, the quasi-periodic Green's function of the Laplace equation are obtained from that of the Helmholtz equation by taking the limit $\sigma \to 0$. We then end up with discussion (section 7) and summary and conclusions (section 8).

To make this paper as readable as possible, several technical arguments have been relegated to a number of appendices. Appendix A summarizes relevant integral representations of $\mathcal{H}_l^+$ and appendix B lists relevant properties of harmonics $\mathcal{Y}_L$. Some useful properties of free-space scattering Green's function are collected in appendix C, whereas appendix D shows several forms of Jacobi identities. Some of the general properties of free-space quasi-periodic Green's functions and the lattice sums are outlined in appendix E. Alternative definitions of lattice sums and structure constants are then summarized in appendix F.

2. Notation and definitions: $G_{0\Lambda}$ and lattice sums

2.1. $G_{0\Lambda}$

A corresponding free-space (quasi-) periodic Green's function $G_{0\Lambda}$ of a scalar Helmholtz equation is defined by an image-like series

$$G_{0\Lambda}(\sigma, \mathbf{k}, \mathbf{R}) = \sum_{\mathbf{r}_n \in \Lambda} G_0^+(\sigma, \mathbf{R} + \mathbf{r}_n)\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_n} = \sum_{\mathbf{r}_n \in \Lambda} G_0^+(\sigma, \mathbf{R} - \mathbf{r}_n)\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_n}, \tag{3}$$

where the origin of coordinates is in the lattice. Here, G_0^+ is the free-space scattering, or retarded, Green's function of a scalar Helmholtz equation in d dimensions,

$$[\Delta + \sigma^2] G_0(\sigma, \mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}'), \tag{4}$$

with Δ being a corresponding Laplace operator, which is represented for large $R = |\mathbf{R}| = |\mathbf{r} - \mathbf{r}'|$ by outgoing waves (i.e., satisfies Sommerfeld radiation condition). Since G_0^+ is only a function of $\mathbf{R} = \mathbf{r} - \mathbf{r}'$, the functional dependence of G_0^+ has been written as $G_0^+(\sigma, \mathbf{R})$ in equation (3). Indeed, G_0^+ is proportional to an appropriate Hankel function of zero order [16]:

$$G_0^+(\sigma, \mathbf{R}) = \lim_{\epsilon \to 0_+} \frac{1}{(2\pi)^d} \int \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}}}{\sigma^2 - k^2 + \mathrm{i}\epsilon}\, \mathrm{d}\mathbf{k} = -\mathrm{i}\frac{\pi}{2} \frac{A}{(2\pi)^d} \sigma^{d-2} \mathcal{H}_0^+(\sigma R) \tag{5}$$

(see also appendix C). Here, $k = |\mathbf{k}|$ and A is the surface of a unit sphere in d dimensions (see equation (B.8)). (With $\mathcal{H}_0(z) = \mathrm{e}^{\mathrm{i}z}$ as a one-dimensional (1D) analogue of the Hankel function [49] equation (5) also becomes valid for $d = 1$, in which case $A = 2$ (unit 'sphere' in 1D consists of two points).) Consequently, upon substituting (5) into (3) one arrives, up to a proportionality factor, to the special case of series (1) for $l = 0$.

A scalar Helmholtz equation is employed for the description of various waves arising in acoustics, mechanics, fluid dynamics, electromagnetism and quantum mechanics [50]. An important class of problems which requires an efficient calculation of $G_{0\Lambda}$ arises in connection with remote sensing of periodic surfaces [25], numerical solution of boundary integral equations for potential flows in fluid mechanics [28–31], periodic gratings, and infinite arrays of resonators coupled to a waveguide [38], in descriptions of dipolar fields in simulated liquid–vapour interfaces [51], in many contexts of simulating systems of charged particles, such as crystal binding and lattice vibrations [9, 11], Madelung constant [11, 12], in various problems in molecular dynamics and Monte Carlo simulations of particles interacting by long-range Coulomb forces [32, 52], wherein periodic boundary conditions are usually imposed in order to avoid the boundary effects.

2.2. Lattice sums

Within a primitive cell of Λ, the respective Green's functions G_0^+ and $G_{0\Lambda}$ only differ up to boundary conditions and their respective singular parts are identical. For the scalar Helmholtz equation, the singular, or principal-value, part of G_0^+ is

$$G_0^p(\sigma,\mathbf{R}) = \mathrm{Re}\, G_0^+(\sigma,\mathbf{R}) = \begin{cases} N_0(\sigma R)/4, & 2D \\ -\cos(\sigma R)/(4\pi R), & 3D \end{cases} \tag{6}$$

where N_0 is the cylindrical Neumann function [16]. Therefore, the difference

$$D_\Lambda(\sigma,\mathbf{k},\mathbf{R}) = G_{0\Lambda}(\sigma,\mathbf{k},\mathbf{R}) - G_0^p(\sigma,\mathbf{R}) \tag{7}$$

is regular for $\mathbf{R}\to 0$ and can be expanded in terms of regular (cylindrical in 2D, spherical in 3D) waves [2, 4, 20, 23, 26, 27, 53]:

$$D_\Lambda(\sigma,\mathbf{k},\mathbf{R}) = \sum_L D_L(\sigma,\mathbf{k})\mathcal{J}_l(\sigma R)\mathcal{Y}_L(\hat{\mathbf{R}}). \tag{8}$$

Here, the symbol $\mathcal{J}_l$ stands for cylindrical and spherical Bessel functions in 2D and 3D, respectively. The expansion coefficients $D_L(\sigma,\mathbf{k})$ introduced by equation (8) are the sought *lattice sums*. The choice of what to subtract in equation (7) is somewhat arbitrary and other choices will lead to slight amended expressions for the lattice sums D_L (see also appendix F). The present choice goes back to Kohn and Rostoker [53] and has been adopted by Ham and Segall [2], Kambe [4, 20], Pendry [22] and others [26, 27].

The series (1) for $l\neq 0$ and $\mathbf{R}\equiv 0$ then formally determine the lattice sums D_L. Indeed, the free-space Green's function is known to possess a partial wave expansion,

$$G_0^+(\sigma,\mathbf{r},\mathbf{r}') = -\mathrm{i}AC\sum_L \mathcal{J}_l(\sigma r_<)\mathcal{H}_l^+(\sigma r_>)\mathcal{Y}_L(\hat{\mathbf{r}}_<)\mathcal{Y}_L^*(\hat{\mathbf{r}}_>), \tag{9}$$

where $r_>$ ($r_<$) is the larger (smaller) of the $|\mathbf{r}|$ and $|\mathbf{r}'|$. The numerical constant C (see equation (10) or equation (C.2)) is basically the prefactor in equation (5). Note that

$$AC = \frac{\pi}{2}\frac{A^2}{(2\pi)^d}\sigma^{d-2} = \begin{cases} \frac{1}{\sigma}, & 1D \\ \frac{\pi}{2}, & 2D \\ \sigma, & 3D. \end{cases} \tag{10}$$

When the partial wave expansion is substituted for G_0^+ in the series (3) for $G_{0\Lambda}$, then, according to equations (7), (8), one has

$$D_L(\sigma,\mathbf{k}) = -\mathrm{i}CA^{1/2}\delta_{L0} - \mathrm{i}AC\sum_{\mathbf{r}_n\in\Lambda}{}'\mathcal{H}_l^+(\sigma r_n)\mathcal{Y}_L^*(\hat{\mathbf{r}}_n)\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_n}, \tag{11}$$

where a prime on summation sign will here and hereafter indicate that the term $\mathbf{r}_n = 0$ is omitted from the sum. Thus as it has been alluded to above, the series (11) is, up to a constant term and a proportionality factor, the special case of series (1) for $l\neq 0$ and $\mathbf{R}=0$.

It is worthwhile to point out that one is often rather interested in the lattice sums D_L than at $G_{0\Lambda}$ itself. For instance, since D_L's do not depend on $\mathbf{R}$, $G_{0\Lambda}$ can be evaluated using equations (7) and (8) at any observation point with the same set of the lattice sums. This can in turn significantly speed up numerical solutions of various boundary-value problems. Knowledge of the lattice sums D_L is a key to efficient numerical analysis of various *ab* *initio* first-principle multiple-scattering problems, such as band structure calculation within Korringa–Kohn–Rostoker (KKR) theories [1, 2, 23, 53–64], and diffraction problems by periodic structures, or gratings, using the so-called layer KKR (LKKR) theories or equivalents thereof, either for quantum (electron) waves within low-energy electron diffraction (LEED) theory [4, 20, 22, 65, 66] or for various classical (acoustic, elastic, electromagnetic, water) waves [5, 26, 64, 67–73]. Lattice sums also arise in quantizing classically ergodic systems such as Sinai's billiard [24] and its various electromagnetic analogues [24, 74]. Moreover, the spectrum within the one-particle theory of periodic point (zero-range) interactions is determined as the set of those z which, for a given $\mathbf{k}_\parallel$ and α, satisfy an implicit equation [13, 47]

$$D_{00}(\mathrm{i}\sqrt{-z}, \mathbf{k}_\parallel) = \tilde{\alpha}. \tag{12}$$

The spectral parameter $\tilde{\alpha}$ here is a boundary-condition parameter which determines the asymptotic of eigenfunctions at the lattice points and is the same for all the eigenfunctions [13, 47, 75].

3. Dual representations of quasi-periodic $G_{0\Lambda}$

Let Λ^* be a corresponding dual (momentum) lattice, i.e., for any $\mathbf{r}_n \in \Lambda$ and $\mathbf{k}_s \in \Lambda^*$ one has $\mathbf{r}_n \cdot \mathbf{k}_s = 2\pi N$, where N is an integer. It is well known that $G_{0\Lambda}$ has an alternative representation as a sum over the dual lattice Λ^*. For example, in the bulk case, i.e., when $d_\Lambda = d$, the dual sum representation of $G_{0\Lambda}$ is

$$G_{0\Lambda}(\sigma, \mathbf{k}, \mathbf{R}) = \frac{1}{v_0} \sum_{\mathbf{k}_s \in \Lambda^*} \frac{\mathrm{e}^{\mathrm{i}(\mathbf{k}+\mathbf{k}_s)\cdot\mathbf{R}}}{\sigma^2 - (\mathbf{k}+\mathbf{k}_s)^2} = \sum_{\mathbf{k}_s \in \Lambda^*} \frac{\psi(\mathbf{k}+\mathbf{k}_s, \mathbf{r})\psi^*(\mathbf{k}+\mathbf{k}_s, \mathbf{r}')}{\sigma^2 - (\mathbf{k}+\mathbf{k}_s)^2}, \tag{13}$$

with eigenfunctions

$$\psi(\mathbf{k}+\mathbf{k}_s, \mathbf{r}) = \frac{1}{\sqrt{v_0}} \mathrm{e}^{\mathrm{i}(\mathbf{k}+\mathbf{k}_s)\cdot\mathbf{r}} \tag{14}$$

normalized to unity in the fundamental (Wigner–Seitz) domain,

$$\int_{\mathrm{WS}} \psi^*(\mathbf{k}+\mathbf{k}_s, \mathbf{r})\psi(\mathbf{k}+\mathbf{k}_{s'}, \mathbf{r})\,\mathrm{d}\mathbf{r} = \delta_{ss'}, \tag{15}$$

with v_0 being the volume of a unit cell of Λ. A dual representation is sometime called an eigenfunction expansion of $G_{0\Lambda}$. Often the respective representations (3) and (13) of $G_{0\Lambda}$ are also called the *spatial-domain* and *spectral-domain* forms, respectively [28, 29, 31, 33, 35].

In the following, the dual sum representation of $G_{0\Lambda}$ in the quasi-periodic case of 1D periodicity in 3D will be derived and its convergence properties will be discussed. However, before proceeding any further, it turns out expedient to provide some supplementary geometrical definitions which are up to minor variations adopted, for instance, within LEED and LKKR theories [4, 20, 22, 26, 27, 65–69, 71–73].

3.1. Supplementary geometrical definitions

In the quasi-periodic case, we define the respective parallel and perpendicular components $\mathbf{r}_\parallel$ and $\mathbf{r}_\perp$ of a given vector $\mathbf{r} = \mathbf{r}_\parallel + \mathbf{r}_\perp$ with respect to the d_Λ-dimensional plane containing the Bravais lattice Λ (i.e., line for $d_\Lambda = 1$ and surface for $d_\Lambda = 2$) and its normal $\mathbf{n}$, respectively. Then for any $\mathbf{r}_n \in \Lambda$,

$$\mathbf{r}\cdot\mathbf{r}_n = \mathbf{r}_\parallel \cdot \mathbf{r}_n, \qquad \mathbf{r}_\perp \cdot \mathbf{r}_n \equiv 0. \tag{16}$$

The respective projections $\mathbf{k}_\parallel$ and $\mathbf{k}_\perp$ of wave vector $\mathbf{k} = \mathbf{k}_\parallel + \mathbf{k}_\perp$ are then defined in like manner with respect to Λ^*. Obviously, in a quasi-periodic case the quantities

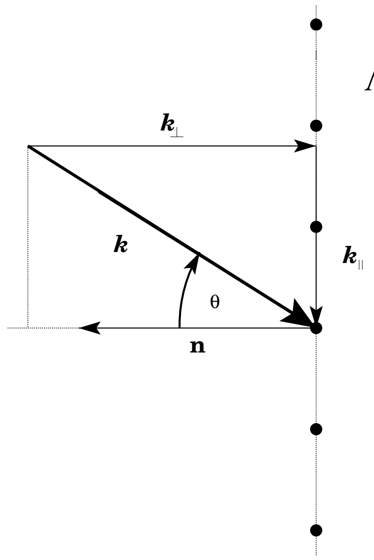

Figure 1. Geometry and parameters—a plane wave with wave vector $\mathbf{k}$ incident on Λ with an incidence angle θ.

$G_{0\Lambda}(\sigma, \mathbf{k}, \mathbf{R})$, $D_\Lambda(\sigma, \mathbf{k}, \mathbf{R})$ and $D_L(\sigma, \mathbf{k})$ entering equations (3), (7), (8), (11) are only functions of $\mathbf{k}_\parallel$. Therefore, in the quasi-periodic case, i.e., if the underlying lattice Λ is of lower dimensionality than the embedding space ($d_\Lambda < d$), it is more appropriate to call merely the projection $\mathbf{k}_\parallel$ as the Bloch momentum.

A plane wave $\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$ incident on a scattering plane of identical scatterers arranged regularly on Λ would (see figure 1), in general, be diffracted (transmitted) to a wave with a wave vector $\mathbf{K}_n^-$ $(\mathbf{K}_n^+)$, where $\mathbf{K}_n^\pm = (\mathbf{k}_\parallel + \mathbf{k}_n, K_{\perp n}^\pm)$,

$$K_{\perp n}^\pm = \pm K_{\perp n} = \begin{cases} \pm[\sigma^2 - |\mathbf{k}_\parallel + \mathbf{k}_n|^2]^{1/2}, & \sigma^2 \geqslant |\mathbf{k}_\parallel + \mathbf{k}_n|^2, \\ \pm\mathrm{i}[|\mathbf{k}_\parallel + \mathbf{k}_n|^2 - \sigma^2]^{1/2}, & \sigma^2 < |\mathbf{k}_\parallel + \mathbf{k}_n|^2, \end{cases} \tag{17}$$

where $\mathbf{k}_n \in \Lambda^*$ and $|\mathbf{k}| = |\mathbf{K}_n^\pm| = \sigma$. Here $K_{\perp n}$ is indicated as a scalar, which is definitely true for $d - d_\Lambda = 1$. In the case of a 1D periodic chain in 3D ($d - d_\Lambda = 2$), $K_{\perp n}$ will be taken as the projection of $\mathbf{K}_{\perp n}$ on the plane spanned by the wave vectors of incident and diffracted beams. In the above definition, the projection $\mathbf{K}_{\parallel n} = \mathbf{k}_\parallel + \mathbf{k}_n$ is real but the normal projection $K_{\perp n}$ can be either real or imaginary. In the case of real $K_{\perp n}$, we speak of a *propagating wave*, and in the case of imaginary $K_{\perp n}$ of an *evanescent wave*.

In the present case the scatterers are absent. Nevertheless, it turns out expedient to define wave vectors $\mathbf{K}_n^\pm$ and the respective projections $\mathbf{K}_{\parallel n}$ and $K_{\perp n}^\pm$ even in the free-space case.

3.2. Resulting series

In order to establish a dual representation of a quasi-periodic $G_{0\Lambda}$ for $d - d_\Lambda = 2$, i.e. a 1D periodicity along the x-axis in 3D, one first substitutes the integral representation (5) of G_0^+ into defining equation (3) of a free-space quasi-periodic Green's function $G_{0\Lambda}$. Then, the Poisson formula

$$\sum_{\mathbf{r}_n \in \Lambda} \mathrm{e}^{\mathrm{i}(\mathbf{q}_\parallel - \mathbf{k}_\parallel)\cdot\mathbf{r}_{\parallel n}} = \frac{(2\pi)^{d_\Lambda}}{v_0} \sum_{\mathbf{k}_n \in \Lambda^*} \delta(\mathbf{q}_\parallel - \mathbf{k}_\parallel - \mathbf{k}_n) \tag{18}$$

is applied resulting in

$$G_{0\Lambda}(\sigma,\mathbf{k}_\parallel,\mathbf{R}) = \frac{(2\pi)^{d_\Lambda-d}}{v_0}\sum_{\mathbf{k}_n\in\Lambda^*}\int \frac{\mathrm{e}^{\mathrm{i}\mathbf{q}_\perp\cdot\mathbf{R}_\perp+\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_n)\cdot\mathbf{R}_\parallel}}{\sigma^2-\mathbf{q}_\perp^2-|\mathbf{k}_\parallel+\mathbf{k}_n|^2+\mathrm{i}\epsilon}\,\mathrm{d}\mathbf{q}_\perp. \tag{19}$$

Now the 2D plane-wave expansion (B.7) is applied to $\mathrm{e}^{\mathrm{i}\mathbf{q}_\perp\cdot\mathbf{R}_\perp}$. Using the orthonormality of cylindrical harmonics $Y_l = \mathrm{e}^{\mathrm{i}l\phi}/\sqrt{2\pi}$, one finds (equation (B.6))

$$\int_0^{2\pi} Y_l(\phi)\,\mathrm{d}\phi = \sqrt{2\pi}\,\delta_{l0}. \tag{20}$$

Therefore, integration in the integral representation (19) of $G_{0\Lambda}$ over $\mathbf{q}_\perp$ results in

$$\begin{aligned} G_{0\Lambda}(\sigma,\mathbf{k}_\parallel,\mathbf{R}) &= \frac{(2\pi)^{d_\Lambda-d+1}}{v_0}\sum_{\mathbf{k}_n\in\Lambda^*}\mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_n)\cdot\mathbf{R}_\parallel}\int_0^\infty \frac{q_\perp J_0(q_\perp|R_\perp|)}{\sigma^2-q_\perp^2-|\mathbf{k}_\parallel+\mathbf{k}_n|^2+\mathrm{i}\epsilon}\,\mathrm{d}q_\perp \\ &= -\frac{\mathrm{i}}{4v_0}\sum_{\mathbf{k}_n\in\Lambda^*}\mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_n)\cdot\mathbf{R}_\parallel} H_0(K_{\perp n}|R_\perp|). \end{aligned} \tag{21}$$

Here in going from the first to second equality the integral identity (C.3) for 2D case has been applied. Thereby, the sum over $\mathbf{r}_n \in \Lambda$ has been transformed into a sum over $\mathbf{k}_n \in \Lambda^*$ resulting in the so-called dual representation (spectral-domain form) of $G_{0\Lambda}$.

3.2.1. Complementary cases. For completeness, in the case of codimension 1 ($d - d_\Lambda = 1$), one first performs a partial integral over $\mathbf{R}_\perp$ in the integral representation (5) of free-space Green's function. This amounts to picking up a residue of a contour integral in the complex plane according to Cauchy theorem resulting in

$$G_0^+(\sigma,\mathbf{R}) = -\frac{\pi\mathrm{i}}{(2\pi)^d}\int \frac{\mathrm{e}^{\mathrm{i}\mathbf{q}_\parallel\cdot\mathbf{R}_\parallel+\mathrm{i}\sqrt{\sigma^2-\mathbf{q}_\parallel^2}|R_\perp|}}{\sqrt{\sigma^2-\mathbf{q}_\parallel^2}}\,\mathrm{d}\mathbf{q}_\parallel. \tag{22}$$

Substituting the integral representation of $G_0^+(\sigma,\mathbf{R})$ into defining equation (3) of a free-space quasi-periodic Green's function $G_{0\Lambda}$ then results in

$$\begin{aligned} G_{0\Lambda}(\sigma,\mathbf{k}_\parallel,\mathbf{R}) &= -\frac{\pi\mathrm{i}}{(2\pi)^d}\int \frac{\mathrm{e}^{\mathrm{i}\mathbf{q}_\parallel\cdot\mathbf{R}_\parallel+\mathrm{i}\sqrt{\sigma^2-\mathbf{q}_\parallel^2}|R_\perp|}}{\sqrt{\sigma^2-\mathbf{q}_\parallel^2}}\left[\sum_{\mathbf{r}_n\in\Lambda}\mathrm{e}^{\mathrm{i}(\mathbf{q}_\parallel-\mathbf{k}_\parallel)\cdot\mathbf{r}_{\parallel n}}\right]\mathrm{d}\mathbf{q}_\parallel \\ &= -\frac{\mathrm{i}}{2v_0}\sum_{\mathbf{k}_n\in\Lambda^*}\frac{\mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_n)\cdot\mathbf{R}_\parallel+\mathrm{i}K_{\perp n}|R_\perp|}}{K_{\perp n}} \\ &= \frac{|R_\perp|}{2v_0}\sum_{\mathbf{k}_n\in\Lambda^*}\mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_n)\cdot\mathbf{R}_\parallel} h_0^{(1)}(K_{\perp n}|R_\perp|), \end{aligned} \tag{23}$$

where $K_{\perp n}$ is given by equation (17). Here in going from the first to second equality the Poisson formula (18) has been applied. Note in passing that the respective dual representations for a 1D periodicity in 2D and 2D periodicity in 3D are formally identical, the only difference being the dimensionality of Λ^* in (23).

Since exponentials in the second equality in (23) can be rewritten as a product of two 'eigenfunctions', the dual representation can be recast in the form of an eigenfunction expansion of $G_{0\Lambda}$ (cf Equation (13)). On the other hand, since $H_0(K_{\perp n}|R_\perp|)$ in equation (21) cannot be factored out as a product of two 'eigenfunctions', an eigenfunction interpretation of a dual representation is obscured for the case of a 1D periodicity in 3D.

3.3. Convergence and limiting cases

Note that, according to equation (17), $K_{\perp n}$ is purely imaginary with positive imaginary part for $|\mathbf{k}_\parallel + \mathbf{k}_n| > \sigma$. For purely imaginary argument $z = \mathrm{i}x$ with $x > 0$ the Hankel functions $H_0^{(1)}(\mathrm{i}x)$ are related to modified Bessel functions $K_0(x)$ (equation (9.6.4) of [16]), whereas $h_0^{(1)}(\mathrm{i}x)$ in the series for $d - d_\Lambda = 2$ are related to modified Bessel functions of third kind $\sqrt{\pi/(2x)}K_{1/2}(x)$ (equation (10.2.15) of [16]). This results in rapidly decaying terms and exponential convergence (see equations (9.7.2) and (10.2.17) of [16]). Exponential convergence can also be directly inferred from the explicit expression for

$$h_0^{(1)}(z) = \frac{\mathrm{e}^{\mathrm{i}z}}{\mathrm{i}z}. \tag{24}$$

One then easily finds that the respective terms in series (23) become exponentially decreasing with increasing $|\mathbf{k}_\parallel + \mathbf{k}_n|$ for $R_\perp \neq 0$. Since $H_0^{(1)}(z) \sim \sqrt{2/(\pi z)}\,\mathrm{e}^{\mathrm{i}(z-\pi/4)}$ for $|z| \to \infty$ and $-\pi < \arg z < 2\pi$ (see equation (9.2.3) of [16], see also equation (2)), the same applies to the series (21). Therefore, although the convergence of a dual representation of Green's function is initially (for $|\mathbf{k}_\parallel + \mathbf{k}_n| \leqslant \sigma$) slow as the series consists of mere oscillating terms, afterward (for $|\mathbf{k}_\parallel + \mathbf{k}_n| > \sigma$) convergence becomes exponential for $R_\perp \neq 0$ (assuming as usual $K_{\perp n} \neq 0$).

Note in passing that all the dual representations of the reduced sums are *nonanalytic* in $R_\perp$ as they are functions of $|R_\perp|$. In the case of series (23), one has

$$|R_\perp| h_0^{(1)}(K_{\perp n}|R_\perp|) \to -\mathrm{i}/K_{\perp n} \qquad \text{as} \quad |R_\perp| \to 0. \tag{25}$$

Therefore, absolute convergence of the resulting series in the limiting case cannot be established even for a 1D periodicity in 2D ([48], pp 51–2). Even worse, in the case of a 1D periodicity in 3D individual terms of the series (21) possess a logarithmic singularity (see equations (9.1.3), (9.1.13) of [16]).

To this end, it has been demonstrated that absolute convergence of dual representations can only be established under the assumption of $R_\perp \neq 0$. Additionally, obtaining the quasi-periodic Green's function of the Laplace equation from that of the Helmholtz equation by taking the limit $\sigma \to 0$ in the resulting expressions (see section 6) is problematic when starting from a dual representation. Since

$$\mathcal{H}_0^+(K_{\perp n}|R_\perp|) \to \mathcal{H}_0^+(\mathrm{i}|\mathbf{k}_\parallel + \mathbf{k}_n||R_\perp|) \qquad \text{as} \quad \sigma \to 0, \tag{26}$$

absolute convergence can again be established only for $R_\perp \neq 0$. In order to resolve the above problems it turns out expedient to invoke representations which converge uniformly and absolutely with respect to $\mathbf{R}$. Such representations are known as the Ewald representations [18, 19]. Additional bonus of the Ewald representations is that they enable one to investigate analytic properties of quasi-periodic Green's functions in the complex variable $z = \sigma^2$.

As a final remark of this section note that dual representations in the quasi-periodic case can also be established by applying an Ewald integral representation of Green's function and the generalized Jacobi identity. This path, which has been originally followed by McRae [76] for a 2D periodicity in 3D, is outlined in the online supplementary material available at stacks.iop.org/JPhysA/39/11247.

4. Ewald representations of quasi-periodic $G_{0\Lambda}$

In going from the spatial-domain form (equation (3)) to the respective spectral-domain forms of $G_{0\Lambda}$ (equations (21), (23)), the summation over Λ has been fully replaced by a summation over Λ^*. In this section, starting from the spectral-domain forms of $G_{0\Lambda}$ a half-step backward will be performed resulting in a hybrid Ewald representation of $G_{0\Lambda}$. The Ewald representation of $G_{0\Lambda}$ involves sums over both Λ and Λ^* and, in contrast to a dual, spectral domain, form of $G_{0\Lambda}$, is valid for all $R_\perp$ and uniformly convergent with respect to bounded sets of $\mathbf{R}$, provided that $\mathbf{R} \not\in \Lambda$.

In deriving the Ewald representation of $G_{0\Lambda}$, we first recall formulae (10.1.1) and (9.1.6) of [16] and recast $h_0^{(1)}$ in the series (23) as

$$h_0^{(1)}(z) = \left(\frac{\pi}{2z}\right)^{1/2} H_{1/2}^{(1)}(z) = -\mathrm{i}\left(\frac{\pi}{2z}\right)^{1/2} H_{-1/2}^{(1)}(z). \tag{27}$$

Therefore, a dual representation of $G_{0\Lambda}$ in any quasi-periodic case (equations (21), (23)) can be rewritten as a sum of *cylindrical* Hankel functions of an appropriate order.

Now for $d - d_\Lambda = 2$, we shall introduce

$$G_{\nu\Lambda}(\sigma, \mathbf{k}, \mathbf{R}) = -\frac{\mathrm{i}}{4v_0} \sum_{\mathbf{k}_n \in \Lambda^*} \left(\frac{|R_\perp|}{K_{\perp n}}\right)^{\nu/2} H_{-\nu/2}^{(1)}(K_{\perp n}|R_\perp|)\, \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel + \mathbf{k}_n)\cdot \mathbf{R}_\parallel}. \tag{28}$$

In the following, $G_{\nu\Lambda}$ will be called an *analytic form* of $G_{0\Lambda}$. Obviously $G_{0\Lambda} = G_{\nu\Lambda}|_{\nu=0}$. Next it turns out expedient to employ the following integral representation (see equation (A.6) of appendix A):

$$\left(\frac{|R_\perp|}{K_{\perp n}}\right)^{\nu/2} H_{-\nu/2}^{(1)}(K_{\perp n}|R_\perp|) = \frac{1}{\pi \mathrm{i}} \int_{0_+}^{\infty \exp \mathrm{i}\phi_n} \zeta^{\nu/2-1}\, \mathrm{e}^{\frac{1}{2}(K_{\perp n}^2 \zeta - |R_\perp|^2/\zeta)}\, \mathrm{d}\zeta. \tag{29}$$

The lower limit 0_+ indicates that the contour integral starts from 0 in the direction of the positive real axis. Here, we have used the convention (see [48], p 589) that

$$\left(\frac{|R_\perp|}{K_{\perp n}}\right)^{\nu/2} = \exp\left\{\frac{\nu}{2}\left(\ln\left|\frac{R_\perp}{K_{\perp n}}\right| - \mathrm{i} \arg K_{\perp n}\right)\right\}, \tag{30}$$

where the argument of $K_{\perp n}$ takes the values 0 or $\pi/2$, and ϕ_n is given by

$$\phi_n = \pi - 2 \arg K_{\perp n}. \tag{31}$$

From equation (29) it follows that $H_0^{(1)}(K_{\perp n}|R_\perp|)$, and hence also $G_{0\Lambda}$, can be analytically continued in the complex parameter ν. This explains the reason why $G_{\nu\Lambda}$ defined by equation (28) has been called an *analytic form* of $G_{0\Lambda}$. Indeed, as soon as $\mathrm{Re}\,\nu > 0$,

$$H_{-\nu/2}^{(1)}(z) \sim -\mathrm{i}\frac{\mathrm{e}^{\nu\pi \mathrm{i}/2}}{\pi} \Gamma(\nu/2)(z/2)^{-\nu/2} \qquad \text{as} \quad z \to 0 \tag{32}$$

(equations (9.1.6) and (9.1.9) of [16]). Therefore, all the terms in the series (28) for $\mathrm{Re}\,\nu > 0$ are singularity free as $|R_\perp| \to 0$, and the original logarithmic singularity of $H_0^{(1)}(K_{\perp n}|R_\perp|)$ in the limit $|R_\perp| \to 0$ in the dual representation (21) of $G_{0\Lambda}$ is thereby avoided. Additionally, the series in (28) can be easily seen as an analytic function of ν for all values of $\mathbf{R}$, provided that $\mathrm{Re}\,\nu > 2d_\Lambda$. In the latter case, upon using asymptotic (32), the elementary products $|R_\perp|^{\nu/2} H_{-\nu/2}^{(1)}(K_{\perp n}|R_\perp|)$ in the series (28) can be uniformly bounded for all n by a *finite* number as $|R_\perp| \to 0$. On the other hand, the asymptotics of $H_{-\nu/2}^{(1)}(z) = \mathrm{e}^{\nu\pi \mathrm{i}/2} H_{\nu/2}^{(1)}(z)$ (equation (9.1.6) of [16]) as $K_{\perp n} \to \infty$ is determined according to equation (2) with $d = 2$. Consequently, the series (28) can be uniformly bounded by the series $K_{\perp n}^{-\nu/2}$ for all $\mathbf{R}$. Now the series $K_{\perp n}^{-\nu/2}$ is absolutely convergent for $\mathrm{Re}\,\nu > 2d_\Lambda$ ([48], pp 51–2). Therefore, since the sum in equation (28) is absolutely and uniformly convergent for all $\mathbf{R}$, it defines an analytic function of ν for all values of $R_\perp$ and $\mathbf{R}_\parallel$ if $\mathrm{Re}\,\nu > 2d_\Lambda$ ([48], section 5.32).

Now, the task is to find an analytic continuation $G_{\nu\Lambda}$ from a domain $\mathrm{Re}\,\nu > 2d_\Lambda$ to a domain containing $\nu = 0$. Here, it has been implicitly assumed (and will be proved later on) that the analytical of $G_{\nu\Lambda}$ defined for $\mathrm{Re}\,\nu > 2d_\Lambda$ by the series (28) will yield our $G_{0\Lambda}$ defined by equation (3). The necessity of an analytic continuation in the quasi-periodic case makes derivation of the Ewald representation of $G_{0\Lambda}$ fundamentally different from that in the bulk case. This analytical continuation procedure is analogous to finding the values of the Riemann ζ-function outside the domain of absolute convergence, $\mathrm{Re}\,\nu \leqslant 1$, of its defining series:

$$\zeta(\nu) = \sum_{n=1}^{\infty} n^{-\nu}. \tag{33}$$

In order to find out an analytic continuation $G_{\nu\Lambda}$ in a domain containing $\nu = 0$, one substitutes (29) back into (28) which results in

$$G_{\nu\Lambda}(\sigma, \mathbf{k}_\parallel, \mathbf{R}) = -\frac{1}{4\pi v_0} \sum_{\mathbf{k}_n\in\Lambda^*}^{K_{\perp n}^2>0} \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_n)\cdot\mathbf{R}_\parallel} \int_{0_+}^{-\infty} \zeta^{\nu/2-1}\, \mathrm{e}^{\frac{1}{2}(K_{\perp n}^2\zeta - |R_\perp|^2/\zeta)}\, \mathrm{d}\zeta$$
$$- \frac{1}{4\pi v_0} \sum_{\mathbf{k}_n\in\Lambda^*}^{K_{\perp n}^2<0} \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_n)\cdot\mathbf{R}_\parallel} \int_{0_+}^{+\infty} \zeta^{\nu/2-1}\, \mathrm{e}^{\frac{1}{2}(K_{\perp n}^2\zeta - |R_\perp|^2/\zeta)}\, \mathrm{d}\zeta. \tag{34}$$

The first sum has only a limited number of terms so that the order of integration and summation can be inverted. By a straightforward generalization of Riemann's method (see [48], p 273), the inversion of integration and summation also holds for the second sum in (34), provided that $\mathrm{Re}\,\nu > 2d_\Lambda$ and if always $\mathrm{Re}\,\zeta > 0$ on the contour of integration [21].

The remaining two steps in the derivation of the Ewald representation are essentially those used by Epstein in an analytic continuation of his zeta functions [10, 11]:

- the resulting contour integral is split into two parts by taking a point η somewhere in the domain $\mathrm{Re}\,\eta > 0$, $|\eta| < \infty$;
- the generalized Jacobi identity (D.4), which is valid for $\mathrm{Re}\,\zeta > 0$, is applied for the part of the integral from 0 to η with $\zeta = 1/(2\xi^2)$, and $\mathbf{r}_s = -\mathbf{r}_s$, yielding

$$\sum_{\mathbf{k}_n\in\Lambda^*} \mathrm{e}^{-(\mathbf{k}_n+\mathbf{k}_\parallel)^2\zeta/2+\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_n)\cdot\mathbf{R}_\parallel} = \frac{v_0}{(2\pi\zeta)^{d_\Lambda/2}} \sum_{\mathbf{r}_n\in\Lambda} \mathrm{e}^{-(\mathbf{R}_\parallel+\mathbf{r}_n)^2/(2\zeta)-\mathrm{i}\mathbf{k}_\parallel\cdot\mathbf{r}_n}. \tag{35}$$

Following the first step, $G_{\nu\Lambda}$ is expressed as the sum of two terms,

$$G_{\nu\Lambda}(\sigma, \mathbf{k}_\parallel, \mathbf{R}) = G_1(\sigma, \mathbf{k}_\parallel, \mathbf{R}) + G_2(\sigma, \mathbf{k}_\parallel, \mathbf{R}), \tag{36}$$

where the respective G_1 and G_2 contributions result from the respective contour integrals over $(0, \eta)$ and (η, ∞). Obviously, although each of the partial integrals depends on η, called the Ewald parameter, their sum does not.

Following the second step, equation (34) is transformed into

$$G_{\nu\Lambda}(\mathbf{R}) = -\frac{1}{4\pi v_0} \int_{\eta}^{-\infty} \sum_{\mathbf{k}_n\in\Lambda^*}^{K_{\perp n}^2>0} \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_n)\cdot\mathbf{R}_\parallel} \zeta^{\nu/2-1}\, \mathrm{e}^{\frac{1}{2}(K_{\perp n}^2\zeta - |R_\perp|^2/\zeta)}\, \mathrm{d}\zeta$$
$$- \frac{1}{4\pi v_0} \int_{\eta}^{+\infty} \sum_{\mathbf{k}_n\in\Lambda^*}^{K_{\perp n}^2<0} \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_n)\cdot\mathbf{R}_\parallel} \zeta^{\nu/2-1}\, \mathrm{e}^{\frac{1}{2}(K_{\perp n}^2\zeta - |R_\perp|^2/\zeta)}\, \mathrm{d}\zeta$$
$$- \frac{1}{(2\pi)^{3/2}} \left(\frac{\pi}{2}\right)^{1/2} \int_0^{\eta} \sum_{\mathbf{r}_n\in\Lambda} \mathrm{e}^{-\mathrm{i}\mathbf{k}_\parallel\cdot\mathbf{r}_n} \zeta^{\nu/2-3/2}\, \mathrm{e}^{\frac{1}{2}[\sigma^2\zeta - (\mathbf{R}+\mathbf{r}_n)^2/\zeta]}\, \mathrm{d}\zeta. \tag{37}$$

The latter expression is an analytic function of ν for all values of ν if $|\mathbf{R}| \neq 0$, or more generally if $\mathbf{R} \notin \Lambda$, and it represents the sought analytic continuation of (28) for $\mathrm{Re}\,\nu \leqslant 2d_\Lambda$.

Note in passing that for $\mathbf{R} \in \Lambda$ analyticity can only be established if $\operatorname{Re}\nu > 1$. Otherwise, the last integral diverges for $\mathbf{r}_n = -\mathbf{R}$.

On putting $\nu = 0$, and hence assuming $\mathbf{R} \notin \Lambda$, inverting again the order of summation and integration (since it can be allowed), and substituting $\zeta \to 1/\zeta$ in the last integral,

$$G_{0\Lambda}(\sigma, \mathbf{k}_\parallel, \mathbf{R}) = -\frac{1}{4\pi v_0} \sum_{\mathbf{k}_n \in \Lambda^*} \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel + \mathbf{k}_n)\cdot \mathbf{R}_\parallel} \int_\eta^{\infty \exp \mathrm{i}\phi_n} \zeta^{-1}\, \mathrm{e}^{\frac{1}{2}(K_{\perp n}^2 \zeta - |R_\perp|^2/\zeta)}\, \mathrm{d}\zeta$$
$$- \frac{1}{4\pi^2} \left(\frac{\pi}{2}\right)^{1/2} \sum_{\mathbf{r}_s \in \Lambda} \mathrm{e}^{-\mathrm{i}\mathbf{k}_\parallel \cdot \mathbf{r}_s} \int_{1/\eta}^{\infty} \zeta^{-1/2}\, \mathrm{e}^{\frac{1}{2}[\sigma^2/\zeta - (\mathbf{R}+\mathbf{r}_s)^2 \zeta]}\, \mathrm{d}\zeta. \tag{38}$$

The restriction $\operatorname{Re}\zeta > 0$ going back to the integral representation (29) can now be removed.

4.1. Complementary cases

For completeness, for $d - d_\Lambda = 1$ one would begin with the analytic form

$$G_{\nu\Lambda}(\sigma, \mathbf{k}_\parallel, \mathbf{R}) = -\frac{\mathrm{i}}{2v_0} \left(\frac{\pi}{2}\right)^{1/2} \sum_{\mathbf{k}_n \in \Lambda^*} \left(\frac{|R_\perp|}{K_{\perp n}}\right)^{\nu/2} H^{(1)}_{-\nu/2}(K_{\perp n}|R_\perp|)\, \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel + \mathbf{k}_n)\cdot \mathbf{R}_\parallel}. \tag{39}$$

Similarly as in the preceding case, $G_{\nu\Lambda}$ defines for $\operatorname{Re}\nu > 2d_\Lambda$ an analytic function of ν for all values of $R_\perp$ and $\mathbf{R}_\parallel$, provided that it remains $\mathbf{R} \notin \Lambda$. The task is now to find an analytic continuation $G_{\nu\Lambda}$ from a domain $\operatorname{Re}\nu > 2d_\Lambda$ to a domain containing $\nu = 1$. After repeating the steps which led from equation (28) to equation (38), on putting $\nu = 1$ and inverting again the order of summation and integration, one finds for $d_\Lambda = 2$, $d = 3$ [4, 20],

$$G_{0\Lambda}(\sigma, \mathbf{k}_\parallel, \mathbf{R}) = -\frac{1}{2\pi v_0} \left(\frac{\pi}{2}\right)^{1/2} \sum_{\mathbf{k}_n \in \Lambda^*} \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel + \mathbf{k}_n)\cdot \mathbf{R}_\parallel} \int_\eta^{\infty \exp \mathrm{i}\phi_n} \zeta^{-1/2}\, \mathrm{e}^{\frac{1}{2}(K_{\perp n}^2 \zeta - |R_\perp|^2/\zeta)}\, \mathrm{d}\zeta$$
$$- \frac{1}{4\pi^2} \left(\frac{\pi}{2}\right)^{1/2} \sum_{\mathbf{r}_s \in \Lambda} \mathrm{e}^{-\mathrm{i}\mathbf{k}_\parallel \cdot \mathbf{r}_s} \int_{1/\eta}^{\infty} \zeta^{-1/2}\, \mathrm{e}^{\frac{1}{2}[\sigma^2/\zeta - (\mathbf{R}+\mathbf{r}_s)^2 \zeta]}\, \mathrm{d}\zeta. \tag{40}$$

Similarly, for $d_\Lambda = 1$, $d = 2$ one arrives (see, e.g., [29]) at

$$G_{0\Lambda}(\sigma, \mathbf{k}_\parallel, \mathbf{R}) = -\frac{1}{2\pi v_0} \left(\frac{\pi}{2}\right)^{1/2} \sum_{\mathbf{k}_n \in \Lambda^*} \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel + \mathbf{k}_n)\cdot \mathbf{R}_\parallel} \int_\eta^{\infty \exp \mathrm{i}\phi_n} \zeta^{-1/2}\, \mathrm{e}^{\frac{1}{2}(K_{\perp n}^2 \zeta - |R_\perp|^2/\zeta)}\, \mathrm{d}\zeta$$
$$- \frac{1}{4\pi} \sum_{\mathbf{r}_s \in \Lambda} \mathrm{e}^{-\mathrm{i}\mathbf{k}_\parallel \cdot \mathbf{r}_s} \int_{1/\eta}^{\infty} \zeta^{-1}\, \mathrm{e}^{\frac{1}{2}[\sigma^2/\zeta - (\mathbf{R}+\mathbf{r}_s)^2 \zeta]}\, \mathrm{d}\zeta. \tag{41}$$

It can be proved directly (see, e.g., appendix 3 of [21]) that Ewald representations (38), (40), (41) satisfy equation (4) and the boundary conditions. Therefore, they are required Green's function, which provides *a posteriori* justification of the outlined analytic continuation procedure.

Since the respective dual representations for a 1D periodicity in 2D and 2D periodicity in 3D are formally identical, the terms involving a sum over reciprocal lattice in equations (40) and (41) are identical. Surprisingly enough, the terms involving a sum over direct lattice in equations (38) and (40) are identical too.

4.2. Ewald versus dual representations

One has (see appendix 1 of [21])

$$\int_\eta^{\infty \exp \mathrm{i}\phi_n} \zeta^{-1/2}\, \mathrm{e}^{\frac{1}{2}(K_{\perp n}^2 \zeta - |R_\perp|^2/\zeta)}\, \mathrm{d}\zeta = -\sqrt{2\pi}\, \frac{\mathrm{e}^{\mathrm{i}K_{\perp n}|R_\perp|}}{\mathrm{i}K_{\perp n}} - \int_{1/\eta}^{\infty} \zeta^{-3/2}\, \mathrm{e}^{\frac{1}{2}(K_{\perp n}^2/\zeta - |R_\perp|^2 \zeta)}\, \mathrm{d}\zeta$$

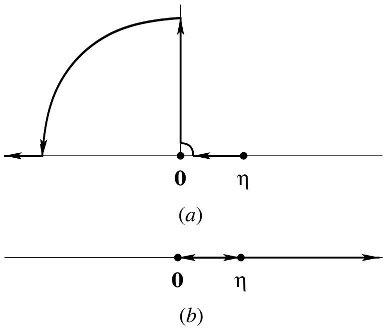

Figure 2. (*a*) Deformation of the integration contour for $K_{\perp n}^2 > 0$ in equations (38), (40), (41) before Jordan's lemma is applied to the quarter circles. (*b*) For $K_{\perp n}^2 < 0$, the integration contour in equations (38), (40), (41) can be considered as a sum of two contours, one from η to zero and the other from zero to $+\infty$.

and

$$\int_\eta^{\infty \exp \mathrm{i}\phi_n} \zeta^{-1}\,\mathrm{e}^{\frac{1}{2}(K_{\perp n}^2\zeta - |R_\perp|^2/\zeta)}\,\mathrm{d}\zeta = \pi\mathrm{i}H_0^{(1)}(K_{\perp n}|R_\perp|) - \int_{1/\eta}^{\infty} \zeta^{-1}\,\mathrm{e}^{\frac{1}{2}(K_{\perp n}^2/\zeta - |R_\perp|^2\zeta)}\,\mathrm{d}\zeta.$$

For $K_{\perp n}^2 > 0$ this can be shown by deforming integration contour in equations (38), (40), (41) to that shown in figure 2(*a*) and upon invoking Jordan's lemma for the integration along quarter circles ([48], p 115). For $K_{\perp n}^2 < 0$ one then takes the contour as shown in figure 2(*b*). Therefore, a comparison of dual representations (21), (23) of quasi-periodic free-space Green's function with their respective Ewald representations (38), (40), (41) shows that to each term of a dual representation the second term (integral above) is added to make the series convergent uniformly with respect to $R_\perp$ (provided that $\mathbf{R} \notin \Lambda$). These terms are then compensated by the series over Λ.

For a sufficiently large η, $G_{0\Lambda}$ can often be well approximated by the series over Λ. This approximation to $G_{0\Lambda}$ is called the *incomplete* Ewald summation [53].

5. Calculation of the lattice sums D_L

The lattice sums D_L have been defined by equation (8) as the expansion coefficients of $G_{0\Lambda}$ in terms of the regular (cylindrical in 2D, spherical in 3D) waves or, alternatively, as the Schlömilch series (11). Analytic closed expression of the lattice sums D_L can only be obtained in the particular case of $l = 0$ and a 1D lattice Λ with a period a in 3D [14, 15]. Indeed, assuming the elementary identity

$$\ln(1 - z) = -\sum_{n>0} \frac{z^n}{n}, \tag{42}$$

one obtains

$$\begin{aligned}\sum_{\mathbf{r}_n \in \Lambda}{}' \mathrm{e}^{\mathrm{i}\mathbf{k}_\parallel \cdot \mathbf{r}_n} \frac{\mathrm{e}^{\mathrm{i}\sigma r_n}}{r_n} &= \frac{1}{a} \sum_{n \neq 0}{}' \mathrm{e}^{\mathrm{i}a\mathbf{k}_\parallel n} \frac{\mathrm{e}^{\mathrm{i}\sigma a|n|}}{|n|} \\ &= -\frac{1}{a}\{\ln[1 - \mathrm{e}^{\mathrm{i}a(\sigma - \mathbf{k}_\parallel)}] + \ln[1 - \mathrm{e}^{\mathrm{i}a(\sigma + \mathbf{k}_\parallel)}]\} \\ &= -\frac{1}{a}\ln[\mathrm{e}^{2\mathrm{i}a\sigma} - 2\cos(\mathbf{k}_\parallel a)\,\mathrm{e}^{\mathrm{i}a\sigma} + 1]. \end{aligned} \tag{43}$$

Hence, upon using that $-\mathrm{i}ACY_{00} = -\mathrm{i}\sigma/\sqrt{4\pi}$ in 3D,

$$D_{00}(\sigma, \mathbf{k}_\parallel) = -\mathrm{i}\frac{\sigma}{\sqrt{4\pi}} + \frac{1}{\sqrt{4\pi}a}\ln[\mathrm{e}^{2\mathrm{i}a\sigma} - 2\cos(\mathbf{k}_\parallel a)\,\mathrm{e}^{\mathrm{i}a\sigma} + 1]$$
$$= \frac{1}{\sqrt{4\pi}a}\ln\{2[\cos(\sigma a) - \cos(\mathbf{k}_\parallel a)]\}, \tag{44}$$

which is up to the prefactor of $-1/(\sqrt{4\pi}a)$, the $\hat{\gamma}$-function of Karpeshina (see equation (29) of [13] for $\sigma = \mathrm{i}s$). (When solving equation (12), the principal branch of logarithm is assumed in the above expression for D_{00} and our spectral parameter $\tilde{\alpha}$ has also been rescaled compared to that of Karpeshina [13, 47] with the above prefactor.) In accordance with our notation, boldface $\mathbf{r}_n$ and $\mathbf{k}_\parallel$ are numbers which can be either positive or negative, whereas $r_n \geqslant 0$ stands for absolute value. (It is recalled here that the energy operator in the one-particle theory of periodic point interactions is constructed in terms of the operator of multiplication by D_{00} (γ function of Karpeshina [13, 47]) and that D_{00} determines the spectrum according to equation (12).)

Invoking that D_L's are independent of R, the lattice sums in all remaining cases are calculated as [4, 20, 26]

$$D_L(\sigma, \mathbf{k}_\parallel) = \lim_{R\to 0}\frac{1}{\mathcal{J}_{|l|}(\sigma R)}\oint \mathcal{Y}_L^*(\hat{\mathbf{R}})D_\Lambda(\sigma, \mathbf{k}_\parallel, \mathbf{R})\,\mathrm{d}\Omega_{\mathbf{R}}, \tag{45}$$

where $\oint \mathrm{d}\Omega_{\mathbf{R}}$ denotes the angular integration over all directions of $\mathbf{R}$. In calculating D_L, the respective Ewald representations (38), (40), (41) of $G_{0\Lambda}$ are substituted in the defining equation (7) for $D_\Lambda(\sigma, \mathbf{k}_\parallel, \mathbf{R})$. The two series in the respective Ewald representations (38), (40), (41) are uniformly convergent with respect to $\mathbf{R}$ so that the series can be termwise integrated when D_L is calculated according to equation (45). Following a hybrid character of the Ewald representations (38), (40), (41), the respective D_L are conventionally written as a sum [2, 4, 20, 26, 27]

$$D_L(\sigma, \mathbf{k}_\parallel) = D_L^{(1)}(\sigma, \mathbf{k}_\parallel) + D_L^{(2)}(\sigma, \mathbf{k}_\parallel) + D_L^{(3)}(\sigma), \tag{46}$$

where $D_L^{(1)}$ $\left(D_L^{(2)}\right)$ involves a sum over reciprocal lattice (all $\mathbf{r}_n \neq 0$ terms of the direct lattice). $D_L^{(3)}$ is the term which combines $G_0^p(\mathbf{R})$ and the $\mathbf{r}_n = 0$ contribution of the direct lattice sum G_2. $D_L^{(3)}$ is only nonzero for $l = 0$,

$$D_L^{(3)} = D_0^{(3)}\delta_{L0}. \tag{47}$$

In the following, the respective contributions $D_L^{(1)}$, $D_L^{(2)}$ and $D_L^{(3)}$ will be calculated. For reader not interested in an explicit derivation of results, the resulting expressions are given by equations (83), (102) and (118) (see equations (85), (102), (118) for $d_\Lambda = 2, d = 3$ and equations (86), (103), (119) for $d_\Lambda = 1, d = 2$).

5.1. Consequences of the reflection symmetry for the lattice sums in the quasi-periodic case

Assuming standard spherical coordinates, one has

$$Y_L(\hat{\mathbf{R}}_\parallel - \hat{\mathbf{R}}_\perp) = (-1)^{l+m}Y_L(\hat{\mathbf{R}}_\parallel + \hat{\mathbf{R}}_\perp). \tag{48}$$

Therefore, for the lattice plane perpendicular to the z-axis

$$D_L \equiv 0, \qquad l + m \text{ odd}, \tag{49}$$

for both $d_\Lambda = 1, d = 3$ and $d_\Lambda = 2, d = 3$ cases. This identity follows upon combining the property (E.2) with the expansion (8). In fact (see equation (47) and equations (67), (100)), it will be shown that (for the lattice plane perpendicular to the z-axis) the property (49) holds for each of the contributions $D_L^{(j)}$, $j = 1, 2, 3$, separately.

5.2. Calculation of $D_L^{(1)}$

5.2.1. General part. As it has been alluded to above, the contribution $D_L^{(1)}$ derives from the sum over reciprocal lattice Λ in the corresponding Ewald representation of $G_{0\Lambda}$. According to the Ewald representations (38), (40), (41) of the quasi-periodic Green's functions,

$$D_L^{(1)} = -\frac{1}{2v_0(2\pi)^c} I_L^{(1)}, \tag{50}$$

where

$$I_L^{(1)} = \lim_{R\to 0} \frac{1}{j_{|l|}(\sigma R)} \oint Y_L^*(\hat{\mathbf{R}})\, \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_s)\cdot\mathbf{R}_\parallel} \int_\eta^{\infty \exp \mathrm{i}\phi_n} \zeta^{-c}\, \mathrm{e}^{\frac{1}{2}(K_{\perp s}^2\zeta - |R_\perp|^2/\zeta)}\, \mathrm{d}\zeta\, \mathrm{d}\Omega_{\mathbf{R}}, \tag{51}$$

and $1/2 \leqslant c = (d-d_\Lambda)/2 \leqslant 1$. The exponential decrease of the integrand with increasing ζ for the integration over ζ (assuming as usual $K_{\perp s} \neq 0$) guarantees that the order of integration can be inverted. In order to perform the latter integral, the exponential is expanded into a power series of $|R_\perp|^2$ resulting in

$$\begin{aligned} I_L^{(1)} &\equiv \sum_{n=0}^{\infty} \frac{(-1)^n}{2^n n!} \int_\eta^{\infty \exp \mathrm{i}\phi_n} \zeta^{-c-n}\, \mathrm{e}^{K_{\perp s}^2 \zeta/2}\, \mathrm{d}\zeta \\ &\quad \times \left(\lim_{R\to 0} \frac{1}{j_{|l|}(\sigma R)} \oint Y_L^*(\hat{\mathbf{R}})\, \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_s)\cdot\mathbf{R}_\parallel} |R_\perp|^{2n}\, \mathrm{d}\Omega_{\mathbf{R}} \right) \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n}{2^n n!} \left(\mathrm{e}^{-\pi \mathrm{i}} \frac{K_{\perp s}^2}{2} \right)^{n+c-1} \Gamma\left(1-c-n, \mathrm{e}^{-\pi\mathrm{i}} \frac{K_{\perp s}^2 \eta}{2}\right) I_\zeta^l(n) \\ &= 2^{1-c}\, \mathrm{e}^{(1-c)\pi\mathrm{i}} \sum_{n=0}^{\infty} \frac{I_\zeta^l(n)}{2^{2n} n!} \Gamma\left(1-c-n, \mathrm{e}^{-\pi\mathrm{i}} \frac{K_{\perp s}^2\eta}{2}\right) K_{\perp s}^{2(n+c-1)}, \end{aligned} \tag{52}$$

where

$$I_\zeta^l(n) = \lim_{R\to 0} \frac{1}{j_{|l|}(\sigma R)} \oint Y_L^*(\hat{\mathbf{R}})\, \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_s)\cdot\mathbf{R}_\parallel} |R_\perp|^{2n}\, \mathrm{d}\Omega_{\mathbf{R}}, \tag{53}$$

and Γ is the incomplete gamma function (see equation (6.5.3) of [16]). In the second equality in (52) we have used in the integral over ζ the substitution

$$\zeta = \frac{2\,\mathrm{e}^{\pi\mathrm{i}}}{K_{\perp s}^2} t, \tag{54}$$

which leads to

$$\begin{aligned} \int_\eta^{\infty \exp \mathrm{i}\phi_n} \zeta^{-c-n}\, \mathrm{e}^{K_{\perp s}^2\zeta/2}\, \mathrm{d}\zeta &= \left(-\frac{2}{K_{\perp s}^2}\right)^{1-c-n} \int_{\mathrm{e}^{-\pi\mathrm{i}} K_{\perp s}^2 \eta/2}^{\infty} t^{-c-n}\, \mathrm{e}^{-t}\, \mathrm{d}t \\ &= \left(-\frac{2}{K_{\perp s}^2}\right)^{1-c-n} \Gamma\left(1-c-n, \mathrm{e}^{-\pi\mathrm{i}} \frac{K_{\perp s}^2 \eta}{2}\right). \end{aligned} \tag{55}$$

In the final equality in (52) we have substituted

$$\left(\mathrm{e}^{-\pi\mathrm{i}} \frac{K_{\perp s}^2}{2}\right)^{n+c-1} = \mathrm{e}^{(1-c)\pi\mathrm{i}} 2^{1-c} \frac{(-1)^n}{2^n} K_{\perp s}^{2(n+c-1)}. \tag{56}$$

Now upon combining equations (50) and (52)

$$\begin{aligned} D_L^{(1)} &= -\frac{1}{(2\pi)^c} \frac{(-2)^{1-c}}{2v_0} \sum_{\mathbf{k}_s \in \Lambda^*} \sum_{n=0}^{\infty} \frac{1}{2^{2n} n!} \Gamma\left(1-c-n, \mathrm{e}^{-\pi\mathrm{i}} \frac{K_{\perp s}^2\eta}{2}\right) K_{\perp s}^{2(n+c-1)} \\ &\quad \times \left(\lim_{R\to 0} \frac{1}{j_{|l|}(\sigma R)} \oint Y_L^*(\hat{\mathbf{R}})\, \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_s)\cdot\mathbf{R}_\parallel} |R_\perp|^{2n}\, \mathrm{d}\Omega_{\mathbf{R}} \right). \end{aligned} \tag{57}$$

It order to finish the calculation of $D_L^{(1)}$, it remains to perform the angular integration and the limit $R \to 0$. In the following, this limit will be performed for various particular cases.

5.2.2. The case of a 1D periodicity in 3D. If the 1D lattice is oriented along the x-axis, $\mathbf{R}_\perp = \mathbf{R}\cos\theta$, $\mathbf{R}_\parallel = \mathbf{R}\sin\theta\cos\phi$, and hence

$$|\mathbf{R}_\perp| = R|\cos\theta|, \qquad (\mathbf{k}_\parallel + \mathbf{k}_s)\cdot\mathbf{R}_\parallel = |\mathbf{k}_\parallel + \mathbf{k}_s|R\sin\theta\cos\left(\phi_{\mathbf{k}_\parallel+\mathbf{k}_s} - \phi\right), \tag{58}$$

where $\phi_{\mathbf{u}}$ is the polar angle of the vector $\mathbf{u}$ in the plane containing Λ^* (Λ). The only difference with respect to the case of a 2D periodicity in 3D, which has been treated by Kambe [4, 20, 21], is merely in that the values of $\phi_{\mathbf{k}_\parallel+\mathbf{k}_s}$ are no longer from the interval $[0, 2\pi)$ but are restricted to either 0 or π. According to equation (52), one has

$$I_L^{(1)} = \mathrm{i}^{m-|m|} N_{l|m|} \sum_{n=0}^{\infty} \frac{1}{2^{2n} n!} \Gamma\left(-n, \mathrm{e}^{-\pi\mathrm{i}} \frac{K_{\perp s}^2 \eta}{2}\right) K_{\perp s}^{2n} \left(\lim_{R\to 0} \frac{R^{2n} I_\Omega^n}{j_l(\sigma R)}\right), \tag{59}$$

where I_Ω^n involves the following angular integral ($\mathrm{d}\Omega = \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$):

$$I_\Omega^n \equiv \int_0^\pi \sin\theta\,\mathrm{d}\theta\, P_l^{|m|}(\cos\theta)(\cos\theta)^{2n} \int_0^{2\pi} \mathrm{e}^{-\mathrm{i}m\phi + \mathrm{i}|\mathbf{k}_\parallel+\mathbf{k}_s|R\sin\theta\cos(\phi_{\mathbf{k}_\parallel+\mathbf{k}_s}-\phi)}\,\mathrm{d}\phi. \tag{60}$$

Integrating first by ϕ, one finds

$$I_\Omega^n = 2\pi\mathrm{i}^{|m|}\,\mathrm{e}^{-\mathrm{i}m\phi_{\mathbf{k}_\parallel+\mathbf{k}_s}} \int_0^\pi P_l^{|m|}(\cos\theta)(\cos\theta)^{2n} J_{|m|}(|\mathbf{k}_\parallel + \mathbf{k}_s|R\sin\theta)\theta\,\mathrm{d}\theta, \tag{61}$$

where we have used that

$$\int_0^{2\pi} \mathrm{e}^{-\mathrm{i}m\phi + \mathrm{i}z\cos(\phi_0-\phi)}\,\mathrm{d}\phi = 2\pi\mathrm{i}^{|m|}\,\mathrm{e}^{-\mathrm{i}m\phi_0} J_{|m|}(z). \tag{62}$$

The latter identity can be derived from (cf equations (9.1.44-45) of [16])

$$\mathrm{e}^{\mathrm{i}z\cos\phi} = \sum_{l=-\infty}^{\infty} \mathrm{i}^{|l|} J_{|l|}(z)\,\mathrm{e}^{\mathrm{i}l\phi}. \tag{63}$$

Since $J_\nu(z)$ is an entire function of z, the Bessel function in equation (61) can be expanded into power series of its argument (see equation (9.1.10) of [16]),

$$J_{|m|}(z) = \left(\frac{z}{2}\right)^{|m|} \sum_{j=0}^{\infty} \frac{(-z^2/4)^j}{j!(|m|+j)!}. \tag{64}$$

Afterward equation (61) becomes

$$I_\Omega^n = 2\pi\mathrm{i}^{|m|}\,\mathrm{e}^{-\mathrm{i}m\phi_{\mathbf{k}_\parallel+\mathbf{k}_s}} \sum_{j=0}^{\infty} (-1)^j \frac{[|\mathbf{k}_\parallel + \mathbf{k}_s|R]^{|m|+2j}}{2^{|m|+2j} j!(|m|+j)!} I_\theta^j, \tag{65}$$

where

$$I_\theta^j \equiv \int_0^\pi (\cos\theta)^{2n}(\sin\theta)^{|m|+2j+1} P_l^{|m|}(\cos\theta)\,\mathrm{d}\theta = \int_{-1}^1 x^{2n}(1-x^2)^{j+|m|/2} P_l^{|m|}(x)\,\mathrm{d}x. \tag{66}$$

It will turn out that, in addition to the general property (49), each term $D_{lm}^{(j)} \equiv 0$, $j = 1, 2, 3$, for $l - |m|$ *odd*. In particular, one can show that the integral (66) vanishes unless $l - |m|$ is *even*, i.e.,

$$D_{lm}^{(1)} \equiv 0, \qquad l - |m| \text{ odd}. \tag{67}$$

Indeed,

$$P_l^{|m|}(\cos\theta) = (-1)^{l-|m|} P_l^{|m|}[\cos(\pi - \theta)]. \tag{68}$$

Now, if F is a real function such that $F(\theta) = F(\pi - \theta)$, then for $l - |m|$ even one finds

$$\int_0^{\pi} F(\theta) P_l^{|m|}(\cos\theta)\,\mathrm{d}\theta = 2\int_0^{\pi/2} F(\theta) P_l^{|m|}(\cos\theta)\,\mathrm{d}\theta. \tag{69}$$

On the other hand, for $l - |m|$ odd the integral vanishes. Since in our case

$$F(\theta) \equiv (\cos\theta)^{2n}(\sin\theta)^{|m|+2j+1} = F(\pi - \theta),$$

it follows that $I_\theta^j \equiv 0$ for $l - |m|$ odd.

For $l - |m|$ even,

$$\lim_{R\to 0} \frac{R^{2n} I_\Omega^n}{j_l(\sigma R)} \to 0, \qquad j + n > \frac{l - |m|}{2}. \tag{70}$$

Therefore, one only needs to investigate the case

$$j + n \leqslant \frac{l - |m|}{2}. \tag{71}$$

Upon expanding $(1 - x^2)^j$ in (66) according to binomial theorem, I_θ^j is rewritten as

$$I_\theta^j = \sum_{s=0}^{j} (-1)^s \binom{j}{s} \int_{-1}^{1} x^{2(n+s)} (1 - x^2)^{|m|/2} P_l^{|m|}(x)\,\mathrm{d}x. \tag{72}$$

According to equation (2.17.2.7) of [77], the integral

$$\int_{-1}^{1} x^t (1 - x^2)^{|m|/2} P_l^{|m|}(x)\,\mathrm{d}x \tag{73}$$

vanishes unless

$$|m| \leqslant l \leqslant t + |m|, \tag{74}$$

or, in our case, unless

$$|m| \leqslant l \leqslant 2n + 2s + |m| \Longleftrightarrow n + s \geqslant \frac{l - |m|}{2}. \tag{75}$$

Upon combining the conditions (71) and (75), it follows that the only nonzero contribution to I_θ^j in the $R \to 0$ limit arises when simultaneously

$$s = j \qquad \text{and} \qquad n + j = \frac{l - |m|}{2}. \tag{76}$$

In the latter case, equation (2.17.2.6) of [77] implies

$$\begin{aligned} I_\theta^j &= (-1)^j \frac{2^{l+1}(2n+2j)!(l+|m|)![n+j+(l+|m|)/2]!}{[n+j-(l-|m|)/2]!(2n+2j+l+|m|+1)!(l-|m|)!} \\ &= (-1)^j \frac{2^{l+1} l!(l+|m|)!}{(2l+1)!}. \end{aligned} \tag{77}$$

Here in the last equation we have substituted for $n + j$ according to equation (76). (Note in passing that equation (2.17.2.6) of [77] differs by a factor $(-1)^m/2$ compared to equation (7.132.5) of [78] due to a slightly different definition of associated Legendre functions.) The constraints (76) imply

$$|m| + 2j = l - 2n, \tag{78}$$

and

$$n \leqslant \frac{l - |m|}{2}. \tag{79}$$

Therefore, the sum over n in $I_L^{(1)}$ becomes a finite sum.

Consequently, as $R \to 0$,

$$R^{2n} I_\Omega^n \sim \mathrm{e}^{-\mathrm{i}m\phi_{\mathbf{k}_\parallel+\mathbf{k}_s}} (-1)^j \frac{2\pi \mathrm{i}^{|m|}[|\mathbf{k}_\parallel + \mathbf{k}_s|]^{l-2n}}{2^{l-2n}[(l-|m|)/2-n]![(l+|m|)/2-n]!} (-1)^j \frac{2^{l+1} l!(l+|m|)!}{(2l+1)!} R^l$$
$$= \mathrm{e}^{-\mathrm{i}m\phi_{\mathbf{k}_\parallel+\mathbf{k}_s}} \frac{2\pi \mathrm{i}^{|m|}[|\mathbf{k}_\parallel + \mathbf{k}_s|]^{l-2n}}{2^{l-2n}[(l-|m|)/2-n]![(l+|m|)/2-n]!} \frac{2^{l+1} l!(l+|m|)!}{(2l+1)!} R^l. \tag{80}$$

Now (equation (10.1.2) of [16])

$$j_l(\sigma R) \to \frac{2^l l!}{(2l+1)!} (\sigma R)^l \qquad (R \to 0). \tag{81}$$

Therefore, in the limit $R \to 0$,

$$I_L^{(1)} = 2\sqrt{\pi} \frac{\mathrm{i}^m}{2^l} [(2l+1)(l+|m|)!(l-|m|)!]^{1/2}\ \mathrm{e}^{-\mathrm{i}m\phi_{\mathbf{k}_\parallel+\mathbf{k}_s}}$$
$$\times \sum_{n=0}^{(l-|m|)/2} \Gamma\left(-n, \mathrm{e}^{-\pi\mathrm{i}} \frac{K_{\perp s}^2 \eta}{2}\right) \frac{[|\mathbf{k}_\parallel + \mathbf{k}_s|/\sigma]^{l-2n}[K_{\perp s}/\sigma]^{2n}}{n![(l-|m|)/2-n]![(l+|m|)/2-n]!}. \tag{82}$$

Consequently, for $l-|m|$ *even*,

$$D_{lm}^{(1)}(\sigma, \mathbf{k}_\parallel) = -\frac{1}{4\pi v_0} I_L^{(1)}$$
$$= -\frac{1}{2\sqrt{\pi} v_0} \frac{\mathrm{i}^m}{2^l} [(2l+1)(l+|m|)!(l-|m|)!]^{1/2} \sum_{\mathbf{k}_s \in \Lambda^*} \mathrm{e}^{-\mathrm{i}m\phi_{\mathbf{k}_\parallel+\mathbf{k}_s}}$$
$$\times \sum_{n=0}^{(l-|m|)/2} \Gamma\left(-n, \mathrm{e}^{-\pi\mathrm{i}} \frac{K_{\perp s}^2 \eta}{2}\right) \frac{[|\mathbf{k}_\parallel + \mathbf{k}_s|/\sigma]^{l-2n}[K_{\perp s}/\sigma]^{2n}}{n![(l-|m|)/2-n]![(l+|m|)/2-n]!}, \tag{83}$$

whereas (equation (67))

$$D_{lm}^{(1)} \equiv 0, \qquad l-|m| \text{ odd}. \tag{84}$$

5.2.3. Complementary cases. For $d_\Lambda = 2$ and $d = 3$, provided that lattice plane is perpendicular to the z-axis, one can repeat most of the steps presented here, the only change being $c = 1/2$ instead of $c = 1$, and thereby arriving at the Kambe's expression [20, 22, 27]

$$D_{lm}^{(1)}(\sigma, \mathbf{k}_\parallel) = -\frac{1}{2v_0\sqrt{2\pi}} I_L^{(1)}$$
$$= -\frac{1}{\sigma v_0} \frac{\mathrm{i}^{-m+1}}{2^l} [(2l+1)(l+|m|)!(l-|m|)!]^{1/2} \sum_{\mathbf{k}_s \in \Lambda^*} \mathrm{e}^{-\mathrm{i}m\phi_{\mathbf{k}_\parallel+\mathbf{k}_s}}$$
$$\times \sum_{n=0}^{(l-|m|)/2} \Gamma\left(1/2-n, \mathrm{e}^{-\pi\mathrm{i}} \frac{K_{\perp s}^2 \eta}{2}\right) \frac{[|\mathbf{k}_\parallel + \mathbf{k}_s|/\sigma]^{l-2n}[K_{\perp s}/\sigma]^{2n-1}}{n![(l-|m|)/2-n]![(l+|m|)/2-n]!}. \tag{85}$$

For $d_\Lambda = 1$ and $d = 2$ one then finds [26]

$$D_l^{(1)}(\sigma, \mathbf{k}_\parallel) = -\frac{\mathrm{i}^{|l|+1}|l|!}{\sqrt{2}\sigma v_0} \sum_{\mathbf{k}_s \in \Lambda^*} \sum_{n=0}^{[|l|/2]} \frac{1}{2^{2n} n!} \Gamma\left(1/2-n, \mathrm{e}^{-\pi\mathrm{i}} \frac{K_{\perp s}^2 \eta}{2}\right)$$
$$\times \frac{[|\mathbf{k}_\parallel + \mathbf{k}_s|/\sigma]^{|l|-2n}[K_{\perp s}/\sigma]^{2n-1}}{(|l|-2n)!} \begin{cases} \exp\left[-\mathrm{i}(|l|-2n)\phi_{\mathbf{k}_\parallel+\mathbf{k}_s}\right], & l \geqslant 0, \\ \exp\left[\mathrm{i}(|l|-2n)\phi_{\mathbf{k}_\parallel+\mathbf{k}_s}\right], & l < 0, \end{cases} \tag{86}$$

where v_0 is now the length of the primitive cell of Λ and $[|l|/2]$ stands for the integral part of $|l|/2$.

5.2.4. Convergence and recurrence relations. In virtue of the asymptotic behaviour

$$\Gamma(a,z) \sim z^{a-1}\,\mathrm{e}^{-z} \qquad \text{as} \quad z \to \infty, \quad |\arg z| < 3\pi/2 \tag{87}$$

(equation (6.5.32) of [16]), it is straightforward to verify that convergence of the series on the rhs of expressions (83), (85), (86) is exponential for sufficiently large $K_{\perp s}$. One can verify that the lattice sums $D_L^{(1)}$ are *dimensionless* for $d = 2$ whereas for $d = 3$ the lattice sums $D_L^{(1)}$ have dimension [1/length] (see discussion below equation (F.4)). From the computational point of view, the incomplete gamma function in final expressions (83), (85), (86) can be derived successively by the recurrence formula [20, 22]

$$b\Gamma(b,x) = \Gamma(b+1,x) - x^b\,\mathrm{e}^{-x}, \tag{88}$$

from the value for $n = 0$:

$$\Gamma(1/2,x) = \begin{cases} \sqrt{\pi} - 2\int_0^{\sqrt{x}} \mathrm{e}^{-t^2}\,\mathrm{d}t = \sqrt{\pi}\,\mathrm{erfc}(\sqrt{x}), & \arg x = 0 \\ \sqrt{\pi} \pm 2\mathrm{i}\int_0^{\sqrt{-x}} \mathrm{e}^{t^2}\,\mathrm{d}t, & \arg x = \mp\pi. \end{cases} \tag{89}$$

5.3. Calculation of $D_L^{(2)}$

5.3.1. General part. As it has been alluded to above, the contribution $D_L^{(2)}$ derives from the sum over direct lattice Λ in the Ewald representation of $G_{0\Lambda}$, but with the term $\mathbf{r}_n = 0$ *excluded*. According to equation (45) taken in combination with the representations (38), (40), (41) of the quasi-periodic Green's functions,

$$D_L^{(2)} = -\frac{(2\pi)^c}{8\pi^2} I_L^{(2)}, \tag{90}$$

where

$$I_L^{(2)} = \int_{1/\eta}^{\infty} \zeta^{-c} \left(\lim_{R\to 0} \frac{1}{\mathcal{J}_{|l|}(\sigma R)} \oint \mathcal{Y}_L^*(\hat{\mathbf{R}})\,\mathrm{e}^{\frac{1}{2}[\sigma^2/\zeta - (\mathbf{R}+\mathbf{r}_s)^2\zeta]}\,\mathrm{d}\Omega_{\mathbf{R}} \right) \mathrm{d}\zeta. \tag{91}$$

Here, $c = 1/2$ for $d = 3$ and $c = 1$ for $d = 2$. Using the plane-wave expansion (B.7), which is also valid for complex arguments (see, e.g., appendix 1 of [4] or appendix A of review by Tong [65]),

$$\mathrm{e}^{-(\mathbf{R}+\mathbf{r}_s)^2\zeta/2} = \mathrm{e}^{-(R^2+r_s^2)\zeta/2}\,\mathrm{e}^{\mathrm{i}(\mathrm{i}\zeta\mathbf{r}_s)\cdot\mathbf{R}} = A\,\mathrm{e}^{-(R^2+r_s^2)\zeta/2} \sum_L \mathrm{i}^{|l|} \mathcal{J}_{|l|}(\mathrm{i}\zeta r_s R) \mathcal{Y}_L^*(\hat{\mathbf{r}}_s) \mathcal{Y}_L(\hat{\mathbf{R}}). \tag{92}$$

The absolute value $|l|$ here is only relevant for $d = 2$ provided that the range of angular momenta is taken to be $-\infty < l < \infty$.

Substituting (92) back into equation for $I_L^{(2)}$, taking the limit (45) and using that in any dimension

$$\frac{\mathcal{J}_l(az)}{\mathcal{J}_l(bz)} \to \frac{a^l}{b^l} \qquad \text{as} \quad z \to 0, \tag{93}$$

$$I_L^{(2)} = A\mathrm{i}^{|l|} \mathcal{Y}_L^*(\hat{\mathbf{r}}_s) \frac{(\mathrm{i}r_s)^{|l|}}{\sigma^{|l|}} \int_{1/\eta}^{\infty} \zeta^{|l|-c}\,\mathrm{e}^{\frac{1}{2}(\sigma^2/\zeta - \mathbf{r}_s^2\zeta)}\,\mathrm{d}\zeta. \tag{94}$$

The substitution

$$\zeta = \frac{\sigma^2}{2u}, \qquad r_s^2\zeta = \frac{\sigma^2 r_s^2}{2u}, \qquad \mathrm{d}\zeta = -\frac{\sigma^2}{2u^2}\,\mathrm{d}u, \qquad \alpha = \frac{\sigma^2\eta}{2}, \tag{95}$$

then yields

$$I_L^{(2)} = A(-1)^{|l|}2^{-|l|-1+c}\sigma^{2-2c}(\sigma r_s)^{|l|}\mathcal{Y}_L^*(\hat{\mathbf{r}}_s)\int_0^\alpha u^{c-|l|-2}\,\mathrm{e}^{u-\sigma^2 r_s^2/(4u)}\,\mathrm{d}u. \tag{96}$$

To this end, the formula for $D_L^{(2)}$ is valid in any quasi-periodic case.

5.3.2. Quasi-periodic cases in 3D. In 3D one has $c = 1/2$ for both 1D and 2D periodicities. Equation (96) then yields

$$I_L^{(2)} = 4\pi(-1)^l 2^{-l-1/2}\sigma(\sigma r_s)^l Y_L^*(\hat{\mathbf{r}}_s)\int_0^\alpha u^{-l-3/2}\,\mathrm{e}^{u-\sigma^2 r_s^2/(4u)}\,\mathrm{d}u. \tag{97}$$

After substituting the result into (90),

$$D_L^{(2)} = -\frac{(-1)^l\sigma}{2^l\sqrt{4\pi}}\sum_{\mathbf{r}_s\in\Lambda}{}' \,\mathrm{e}^{-\mathrm{i}\mathbf{k}_\parallel\cdot\mathbf{r}_s}(\sigma r_s)^l Y_L^*(\hat{\mathbf{r}}_s)\int_0^\alpha u^{-l-3/2}\,\mathrm{e}^{u-\sigma^2 r_s^2/(4u)}\,\mathrm{d}u, \tag{98}$$

where prime in $\sum'$ indicates as usual that the term with $r_s = 0$ is omitted. Since, for $l+m$ *odd*,

$$Y_{lm}(\pi/2,\phi) \equiv 0, \tag{99}$$

$$D_L^{(2)} \equiv 0, \qquad l+m \text{ odd}. \tag{100}$$

(We recall here that the periodicity direction(s) has (have) been assumed to be perpendicular to the z-axis.) This confirms (see equation (67)) that, in addition to the general property (49), each term $D_{lm}^{(j)} \equiv 0$, $j = 1, 2, 3$, for $l - |m|$ *odd*. In the remaining cases for $l+m$ *even* [4, 20, 22],

$$Y_{lm}^*(\pi/2,\phi) = (-1)^{(m-|m|)/2}\frac{(-1)^{(l+|m|)/2}}{2^l\sqrt{4\pi}}\frac{[(2l+1)(l-|m|)!(l+|m|)!]^{1/2}}{[(l-|m|)/2]![(l+|m|)/2]!}\,\mathrm{e}^{-\mathrm{i}m\phi}. \tag{101}$$

Therefore,

$$\begin{aligned} D_{lm}^{(2)}(\sigma,\mathbf{k}_\parallel) = {}& -\frac{\sigma}{4\pi}\frac{(-1)^l(-1)^{(l+m)/2}}{2^{2l}}\frac{[(2l+1)(l-|m|)!(l+|m|)!]^{1/2}}{[(l-|m|)/2]![(l+|m|)/2]!} \\ & \times \sum_{\mathbf{r}_s\in\Lambda}{}' \,\mathrm{e}^{-\mathrm{i}\mathbf{k}_\parallel\cdot\mathbf{r}_s - \mathrm{i}m\phi_{\mathbf{r}_s}}(\sigma r_s)^l\int_0^\alpha u^{-l-3/2}\exp\left[u-\frac{\sigma^2 r_s^2}{4u}\right]\mathrm{d}u, \end{aligned} \tag{102}$$

where $\alpha = \sigma^2\eta/2$ (see equation (95)). Hence, the respective expressions for $D_{lm}^{(2)}$, for $d_\Lambda = 1, d = 3$ and for $d_\Lambda = 2, d = 3$ [20, 22, 27], are formally identical (provided that periodicity direction(s) is (are) perpendicular to the z-axis), the only difference being in the lattice dimension.

5.3.3. Complementary case of a 1D periodicity in 2D. In the remaining case for $d_\Lambda = 1$ and $d = 2$, in which case $c = 1$, one finds by a slight modification of the preceding derivation [26]

$$D_l^{(2)}(\sigma,\mathbf{k}_\parallel) = -\frac{(-1)^{|l|}}{2^{|l|+1}\sqrt{2\pi}}\sum_{\mathbf{r}_s\in\Lambda}{}' \,\mathrm{e}^{-\mathrm{i}\mathbf{k}_\parallel\cdot\mathbf{r}_s}(\sigma r_s)^{|l|}\,\mathrm{e}^{-\mathrm{i}l\phi_{\mathbf{r}_s}}\int_0^\alpha u^{-|l|-1}\exp\left(u-\frac{\sigma^2 r_s^2}{4u}\right)\mathrm{d}u. \tag{103}$$

5.3.4. Convergence and recurrence relations. Similarly as in the case of $D_L^{(1)}$, convergence of the series for $D_L^{(2)}$ on the rhs of expressions (102), (103) is exponential for sufficiently large r_s. Indeed, integrals

$$U_{|l|} = \int_0^\alpha u^{c-|l|-2}\, \mathrm{e}^{u-\sigma^2 r_s^2/(4u)}\, \mathrm{d}u \tag{104}$$

are finite integrals. Now, for $|\sigma r_s| > |l| + 2 - c$, the integrand is monotonically increasing from zero to $(\sigma^2\eta/2)^{c-|l|-2}\, \mathrm{e}^{\sigma^2\eta/2 - r_s^2/(2\eta)}$ on the integration interval. Therefore,

$$|(\sigma r_s)^{|l|} U_{|l|}| < \sigma^{2(c-1)-|l|}(\eta/2)^{c-|l|-1} r_s^{|l|}\, \mathrm{e}^{\sigma^2\eta/2 - r_s^2/(2\eta)}. \tag{105}$$

From the computational point of view, the integral on the rhs of the resulting expressions can easily be performed by a simple recurrence. Indeed, knowing the values of U_0 and U_1, the respective integrals $U_{|l|}$ can be determined using recursion relation

$$\left(\frac{\sigma r_s}{2}\right)^2 U_{|l|+1} = (|l| + 1 - c)U_{|l|} - U_{|l|-1} + \alpha^{-|l|-1+c}\, \mathrm{e}^{\alpha - \sigma^2 r_s^2/(4\alpha)}. \tag{106}$$

The recurrence here follows, as suggested by Kambe (see appendix 2 of [4]), from a simple integration by parts.

As a consistency check, note that for $d = 2$ the lattice sums $D_L^{(2)}$ are *dimensionless*, whereas for $d = 3$ the lattice sums $D_L^{(2)}$ have dimension [1/length] (see discussion below equation (F.4)).

5.4. Calculation of $D_L^{(3)}$

5.4.1. General part. According to equation (47), the only nonzero term is $D_{00}^{(3)}$ or, for the sake of notation, $D_0^{(3)}$. In 3D, for both 1D and 2D periodicities, the $D_0^{(3)}$ term is calculated as the limit

$$D_0^{(3)} = \lim_{R\to 0} \frac{1}{\mathcal{J}_0(\sigma R)\mathcal{Y}_0}\left[-\frac{1}{4\pi^2}\left(\frac{\pi}{2}\right)^{1/2}\int_{1/\eta}^\infty \zeta^{-1/2}\, \mathrm{e}^{\frac{1}{2}(\sigma^2/\zeta - \mathbf{R}^2\zeta)}\, \mathrm{d}\zeta - G_0^p(\sigma, \mathbf{R})\right]. \tag{107}$$

Similarly, in 2D case

$$D_0^{(3)} = \lim_{R\to 0} \frac{1}{\mathcal{J}_0(\sigma R)\mathcal{Y}_0}\left[-\frac{1}{4\pi}\int_{1/\eta}^\infty \zeta^{-1}\, \mathrm{e}^{\frac{1}{2}(\sigma^2/\zeta - \mathbf{R}^2\zeta)}\, \mathrm{d}\zeta - G_0^p(\sigma, \mathbf{R})\right]. \tag{108}$$

It is recalled here that $G_0^p(\sigma, \mathbf{R})$ in equations (107) and (108) is the corresponding singular, or principal-value, part of $G_0^+(\sigma, \mathbf{R})$ (see equation (6)).

In any dimension $\mathcal{Y}_0 = A^{-1/2}$ (equation (B.5)), where A is given by equation (B.8), and (see equations (9.1.12), (10.1.11) of [16])

$$\mathcal{J}_0(\sigma R) \to 1 \qquad (R \to 0). \tag{109}$$

Hence, calculation of $D_0^{(3)}$ requires to perform integral

$$I^{(3)} = \int_{1/\eta}^\infty \zeta^{-c}\, \mathrm{e}^{\frac{1}{2}(\sigma^2/\zeta - \mathbf{R}^2\zeta)}\, \mathrm{d}\zeta \tag{110}$$

for either $c = 1/2$ ($d = 3$) or $c = 1$ ($d = 2$). Expanding $\mathrm{e}^{\sigma^2/(2\zeta)}$ into power series and integrating term by term yields

$$I^{(3)} = \sum_{n=0}^\infty \frac{\sigma^{2n}}{2^n n!}\int_{1/\eta}^\infty \zeta^{-c-n}\, \mathrm{e}^{-\mathbf{R}^2\zeta/2}\, \mathrm{d}\zeta. \tag{111}$$

Since all terms in the sum are positive, the exchange of integration and summation is justified whenever one shows that one of the sides exists (this will be shown later on). Upon substituting $\zeta = 2t/R^2$,

$$I^{(3)} = (R^2/2)^{c-1} \sum_{n=0}^{\infty} \frac{(\sigma^2 R^2)^n}{2^{2n} n!} \int_{R^2/(2\eta)}^{\infty} t^{-c-n}\, \mathrm{e}^{-t}\, \mathrm{d}t$$
$$= (R^2/2)^{c-1} \sum_{n=0}^{\infty} \frac{(\sigma R)^{2n}}{2^{2n} n!} \Gamma[-n-c+1, R^2/(2\eta)],$$

where as usual $\Gamma(a, x)$ is an incomplete gamma function (see equation (6.5.3) of [16]). According to equations (107) and (108), we are only interested in the limit $R \to 0$. For $n > 1 - c$, which for a given $c = 1/2$, 1 translates into $n \geqslant 1$, one can integrate by parts, yielding

$$\int_{R^2/(2\eta)}^{\infty} t^{-c-n}\, \mathrm{e}^{-t}\, \mathrm{d}t = \frac{1}{n+c-1} \left(\frac{R^2}{2\eta}\right)^{-c-n+1} \mathrm{e}^{-R^2/(2\eta)} + \mathcal{O}[R^{-2(c+n-2)}]. \tag{112}$$

Therefore,

$$I^{(3)} = \sum_{n=1}^{\infty} \frac{1}{n+c-1} \frac{(\sigma^2\eta)^n}{2^n n!} + (R^2/2)^{c-1} \int_{R^2/(2\eta)}^{\infty} t^{-c}\, \mathrm{e}^{-t}\, \mathrm{d}t + \mathcal{O}(R^2). \tag{113}$$

A further treatment differs in different dimensions.

5.4.2. Quasi-periodic cases in 3D. In 3D one has $c = 1/2$ for both 1D and 2D periodicities. Hence,

$$\int_{R^2/(2\eta)}^{\infty} t^{-c}\, \mathrm{e}^{-t}\, \mathrm{d}t = \left(\int_0^{\infty} - \int_0^{R^2/(2\eta)}\right) t^{-1/2}\, \mathrm{e}^{-t}\, \mathrm{d}t$$
$$= \Gamma(1/2) - 2\frac{R}{(2\eta)^{1/2}}\, \mathrm{e}^{-R^2/(2\eta)} + \mathcal{O}(R^3), \tag{114}$$

where $\Gamma(1/2) = \sqrt{\pi}$. This asymptotic is consistent with that obtained by writing

$$\Gamma[1/2, R^2/(2\eta)] = \int_{R^2/(2\eta)}^{\infty} t^{-1/2}\, \mathrm{e}^{-t}\, \mathrm{d}t = \sqrt{\pi}\, \mathrm{erfc}(R/\sqrt{2\eta}) \tag{115}$$

(see equation (6.5.17) of [16]) and using that

$$\mathrm{erfc}\, z = 1 - \frac{2z}{\sqrt{\pi}} + \mathcal{O}(z^2) \qquad \text{as} \quad z \to 0 \tag{116}$$

(see equation (7.2.4) of [16]). Therefore,

$$I^{(3)} = \frac{\sqrt{2\pi}}{R} + \frac{\sigma}{\sqrt{2}} \sum_{n=0}^{\infty} \frac{(\sigma^2\eta/2)^{n-1/2}}{n!(n-1/2)} + \mathcal{O}(R^2) \qquad \text{as} \quad R \to 0. \tag{117}$$

Collecting everything together back to equation (107) and taking the limit, the singular first term in $I^{(3)}$ cancels against $G_0^p(\sigma, \mathbf{R})$ leaving behind

$$D_{lm}^{(3)}(\sigma) = -\frac{\sigma}{4\pi} \sum_{n=0}^{\infty} \frac{(\sigma^2\eta/2)^{n-1/2}}{n!(n-1/2)} \delta_{lm,00}. \tag{118}$$

It is emphasized here that the respective contributions $D_{lm}^{(3)}$ for a 1D periodicity in 3D and a 2D periodicity in 3D (see [20, 22, 27]) are identical.

5.4.3. Complementary case of 1D periodicity in 2D. For $d_\Lambda = 1$ and $d = 2$, in which case $c = 1$, one finds [26]

$$D_l^{(3)}(\sigma) = -\frac{1}{2\sqrt{2\pi}}\left[\gamma + \ln(\sigma^2\eta/2) + \sum_{n=1}^{\infty}\frac{(\sigma^2\eta/2)^n}{n!n}\right]\delta_{l0} = \frac{1}{2\sqrt{2\pi}}\mathrm{Ei}(\sigma^2\eta/2)\delta_{l0}, \tag{119}$$

where Ei is an exponential integral and $\gamma \approx 0.577\,215\,6649$ is the Euler constant (see equations (5.1.10) and (6.1.3) of [16], respectively). Note that, for Λ oriented along the x-axis, $D_l^{(j)} = D_{-l}^{(j)}$, $j = 1, 2$, and hence, $D_l = D_{-l}$, in accord with the fact that $G_{0\Lambda}$ only depends on y via $|y|$ [33, 35].

5.4.4. Convergence. Unlike preceding cases, convergence of series on the rhs of equations (118) and (119) is even faster than exponential. This can easily be verified by using Stirling's formula (equation (6.1.37) of [16])

$$(n+1)! \sim \sqrt{2\pi n}n^n\,\mathrm{e}^{-n} \qquad \text{as} \quad n \to \infty. \tag{120}$$

Again, as a consistency check, note that for $d = 2$ the lattice sums $D_L^{(3)}$ are *dimensionless*, whereas for $d = 3$ the lattice sums $D_L^{(3)}$ have dimension [1/length] (see discussion below equation (F.4)). It is recalled here that η in the above formulae has dimension of [length]^2.

6. Laplace equation

The quasi-periodic solutions of the Laplace equation are used to describe potential flows in fluid dynamics between parallel planes and in rectangular channels [30]. Indeed, a Green's function representing a point source and satisfying the respective von Neumann and Dirichlet boundary conditions on a flow channel walls can be written as a sum and difference of an appropriate $G_{0\Lambda}$ (corresponding to 1D periodicity in 3D for the flow between parallel planes and to 2D periodicity in 3D for the flow in a rectangular channel) taken at two different spatial points [30]. Another important class of problems associated with the quasi-periodic solutions of Laplace equation arises in various problems in electrostatics and elastostatics [43, 44, 46].

The relevant representations of $G_{0\Lambda}$ for the Laplace equation can in principle be obtained by taking the limit $\sigma \to 0$ in the resulting expressions for the Helmholtz equation. In 3D, $h_0^{(1)}(\sigma|\mathbf{r} - \mathbf{r}' + \mathbf{r}_s|)$ in the Schlömilch series (1) exhibits a regular limit

$$h_0^{(1)}(\sigma|\mathbf{r} - \mathbf{r}' + \mathbf{r}_s|) \to -\frac{\mathrm{i}}{|\mathbf{r} - \mathbf{r}' + \mathbf{r}_s|} \qquad \text{as} \quad \sigma \to 0 \tag{121}$$

(see equation (24)) and corresponding $G_0^+(\sigma, R)$ goes smoothly to the free-space Green's function of 3D Laplace equation. However, $H_0^{(1)}(\sigma|\mathbf{r} - \mathbf{r}' + \mathbf{r}_s|)$ displays a logarithmic singularity in the same limit (see equations (9.1.3), (9.1.13) of [16]). Hence, $G_0^+(\sigma, R)$ does not reduce to the free-space Green's function $G_0^+(R) = (1/2\pi)\ln R$ of 2D Laplace equation. Surprisingly enough, in the case of dual and Ewald representations of $G_{0\Lambda}$ the logarithmic singularities cooperate in such a way that the limit $\sigma \to 0$ turns out to be regular even for $d = 2$ (see below).

In the following, the limit $\sigma \to 0$ will be discussed in the case of dual and Ewald representations of $G_{0\Lambda}$, and in the case of lattice sums D_{00} in 3D. In taking the limit, both $G_{0\Lambda}$ and D_{00} will be considered formally as functions of two independent variables σ and $\mathbf{k}_\parallel$. A reason for doing so is, for instance, solving an implicit equation (12). The limit $\mathbf{k}_\parallel \to 0$ will be, if possible, considered afterwards.

Note that the case of 1D periodicity with period a in the x-direction in 2D is rather academic in what follows, since in the latter case the Green's function can be calculated in a closed form [30]

$$G_{0\Lambda}(\mathbf{R}) = \frac{1}{\pi}\ln\left[2\left|\sin\frac{\pi}{a}(x+\mathrm{i}y)\right|\right]. \tag{122}$$

6.1. Dual representations

Since $K_{\perp n} \to \mathrm{i}|\mathbf{k}_\parallel + \mathbf{k}_n|$ in the limit $\sigma \to 0$ (cf equation (17)), in all quasi-periodic cases the limit is established (see equation (26)) by replacing $\mathcal{H}_0^+(K_{\perp n}|R_\perp|)$ in equations (21), (23) with $\mathcal{H}_0^+(\mathrm{i}|\mathbf{k}_\parallel + \mathbf{k}_n\|R_\perp|)$. However, for purely imaginary argument $\mathrm{i}x$ with $x > 0$ the Hankel functions $\mathcal{H}_0^+(\mathrm{i}x)$ are related to modified Bessel functions of third kind (see equations (9.6.4) and (10.2.15) of [16]). This results in rapidly decaying terms and exponential convergence. As it has been alluded to earlier, absolute exponential convergence of the dual representations can only be established under the assumption of $R_\perp \neq 0$.

However, the resulting dual representations are singular in the limit $\mathbf{k}_\parallel \to 0$. Then, $K_{\perp n} \to ik_n$ and the denominator in equations (21), (23) vanishes for $\mathbf{k}_n = 0$.

6.2. Ewald representations

The $\sigma \to 0$ limit can also be easily taken in the respective Ewald integral representations (38), (40), (41) of free-space quasi-periodic Green's functions: simply substitute in the above expressions $\phi_n \equiv 0$ and $K_{\perp n}^2 = -|\mathbf{k}_\parallel + \mathbf{k}_n|^2$. Using that the integrals in the series over Λ can be expressed in the $\sigma \to 0$ limit in terms of incomplete gamma functions (equation (6.5.3) of [16]), one finds for the respective Ewald representations (38), (40), (41) the following expressions:

$$\begin{aligned} G_{0\Lambda}(\mathbf{k}_\parallel, \mathbf{R}) = &-\frac{1}{4\pi v_0}\sum_{\mathbf{k}_n\in\Lambda^*} \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_n)\cdot\mathbf{R}_\parallel}\int_\eta^\infty \zeta^{-1}\,\mathrm{e}^{-\frac{1}{2}(|\mathbf{k}_\parallel+\mathbf{k}_n|^2\zeta+|R_\perp|^2/\zeta)}\,\mathrm{d}\zeta \\ &-\frac{1}{4\pi^2}\left(\frac{\pi}{2}\right)^{1/2}\sum_{\mathbf{r}_s\in\Lambda}\mathrm{e}^{-\mathrm{i}\mathbf{k}_\parallel\cdot\mathbf{r}_s}\frac{\sqrt{2}\Gamma[1/2, |\mathbf{R}+\mathbf{r}_s|^2/(2\eta)]}{|\mathbf{R}+\mathbf{r}_s|} \end{aligned} \tag{123}$$

for 1D in 3D,

$$\begin{aligned} G_{0\Lambda}(\mathbf{k}_\parallel, \mathbf{R}) = &-\frac{1}{2\pi v_0}\left(\frac{\pi}{2}\right)^{1/2}\sum_{\mathbf{k}_n\in\Lambda^*} \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_n)\cdot\mathbf{R}_\parallel}\int_\eta^\infty \zeta^{-1/2}\,\mathrm{e}^{-\frac{1}{2}(|\mathbf{k}_\parallel+\mathbf{k}_n|^2\zeta+|R_\perp|^2/\zeta)}\,\mathrm{d}\zeta \\ &-\frac{1}{4\pi^2}\left(\frac{\pi}{2}\right)^{1/2}\sum_{\mathbf{r}_s\in\Lambda}\mathrm{e}^{-\mathrm{i}\mathbf{k}_\parallel\cdot\mathbf{r}_s}\frac{\sqrt{2}\Gamma[1/2, |\mathbf{R}+\mathbf{r}_s|^2/(2\eta)]}{|\mathbf{R}+\mathbf{r}_s|} \end{aligned} \tag{124}$$

for 2D in 3D and

$$\begin{aligned} G_{0\Lambda}(\mathbf{k}_\parallel, \mathbf{R}) = &-\frac{1}{2\pi v_0}\left(\frac{\pi}{2}\right)^{1/2}\sum_{\mathbf{k}_n\in\Lambda^*} \mathrm{e}^{\mathrm{i}(\mathbf{k}_\parallel+\mathbf{k}_n)\cdot\mathbf{R}_\parallel}\int_\eta^\infty \zeta^{-1/2}\,\mathrm{e}^{-\frac{1}{2}(|\mathbf{k}_\parallel+\mathbf{k}_n|^2\zeta+|R_\perp|^2/\zeta)}\,\mathrm{d}\zeta \\ &-\frac{1}{4\pi}\sum_{\mathbf{r}_s\in\Lambda}\mathrm{e}^{-\mathrm{i}\mathbf{k}_\parallel\cdot\mathbf{r}_s}\Gamma[0, |\mathbf{R}+\mathbf{r}_s|^2/(2\eta)] \end{aligned} \tag{125}$$

for 1D in 2D. The Laplace limit of the respective Ewald integral representations then follows straightforwardly by letting $\mathbf{k}_\parallel \to 0$ in the above expressions (123)–(125).

Regarding convergence speed, in virtue of the asymptotic $\Gamma(a,z) \sim z^{a-1}\,\mathrm{e}^{-z}$ for $z \to \infty$, $|\arg z| < 3\pi/2$ (equation (6.5.32) of [16]), the respective Ewald representations remain to be exponentially convergent in the $\sigma \to 0, \mathbf{k}_\parallel \to 0$ limit. Note in passing that $\Gamma[1/2, |\mathbf{R}+\mathbf{r}_s|^2/(2\eta)]$ in equations (123), (124) can be expressed via error function (equation (115)) as

$$\Gamma[1/2, |\mathbf{R}+\mathbf{r}_s|^2/(2\eta)] = \sqrt{\pi}\,\mathrm{erfc}(|\mathbf{R}+\mathbf{r}_s|/\sqrt{2\eta}) \tag{126}$$

(equation (6.5.17) of [16]). An alternative exponentially convergent series for $G_{0\Lambda}$ for 1D periodicity in 3D in the Laplace case has also been obtained earlier by Linton (see series in equation (3.26) of [30]). However, our expressions have been derived without any artificial regularization in the form of a convergence ensuring logarithmically divergent series (cf [30]).

Additionally, absolute exponential convergence of the respective Ewald representations can also be established for $R_\perp = 0$, which for numerous alternative representations of $G_{0\Lambda}$ in fluid dynamics provides a problem [30]. Again, the case $R_\perp = 0$ can only be attained when $\mathbf{R}_\parallel \notin \Lambda$. Otherwise the respective Ewald representations become singular. In 3D this singularity is explicit, since for some $\mathbf{r}_s \in \Lambda$ the denominator $|\mathbf{R}+\mathbf{r}_s|$ vanishes. For 1D in 2D one has $\Gamma[0, |\mathbf{R}+\mathbf{r}_s|^2/(2\eta)] \to \Gamma(0)$ for some $\mathbf{r}_s \in \Lambda$, and the singular behaviour follows from the pole of the gamma function $\Gamma(z)$ for $z = 0$ or more precisely from the asymptotic (equations (6.5.15), (5.1.11) of [16])

$$\Gamma(0, z) = E_1(z) \sim -\gamma - \ln z - \sum_{n=1}^{\infty} \frac{(-z)^n}{nn!} \qquad \text{as} \quad z \to 0, \tag{127}$$

where γ is the Euler constant (equation (6.1.3) of [16]).

As a final remark, note in passing that each of the above Ewald integral representations (123)–(125) can be regarded as a one-parametric continuous spectrum of the representations for $G_{0\Lambda}$. The corresponding dual representations of section 6.1 for $\mathbf{k}_\parallel \neq 0$ can be then recovered in the limit $\eta \to 0$. Indeed, using Hobson's integral representation (A.7), the integrals in the series over Λ^* can be expressed in the limit $\eta \to 0$ in terms of the modified Bessel functions of the third kind $\mathcal{K}_0$ (K_0 for $d - d_\Lambda = 2$ and $K_{1/2}$ for $d - d_\Lambda = 1$).

6.3. Lattice sums in 3D for $l = 0$

In the case of lattice sums D_L, they are defined as expansion coefficients of free-space quasi-periodic Green's functions in terms of regular cylindrical (in $2D$ or spherical (in $3D$) waves $\mathcal{J}_l(\sigma R)\mathcal{Y}_L(\hat{\mathbf{R}})$ (see equation (8))). Since unless $l = 0$ one has $\mathcal{J}_l(\sigma R) \to 0$ in the limit $\sigma \to 0$ (see equation (109)), the lattice sums D_L become singular in the limit for $l \neq 0$. In the case of $l = 0$, it is recalled here that D_{00} (γ function of Karpeshina [13, 47]) determines the energy operator in the one-particle theory of periodic point (zero-range) interactions and that the D_{00} determines the underlying spectrum according to equation (12).

From a mathematical point of view, upon substituting (24) for $\mathcal{H}_0^+$ into (11) and assuming for a while an *integer lattice*, the lattice sum D_L for $l = 0$ in 3D can be expressed in the limit $\sigma \to 0$ via *Epstein zeta function* [9–11]

$$Z\begin{vmatrix} 0 \\ \mathbf{k}_\parallel \end{vmatrix}(\chi, \nu) \equiv \sum_{\mathbf{r}_n \in \Lambda}{}' \frac{\mathrm{e}^{i\mathbf{k}_\parallel \cdot \mathbf{r}_n}}{|\mathbf{r}_n|^\nu} \tag{128}$$

as

$$D_{00}(0, \mathbf{k}_\parallel) = -\frac{1}{\sqrt{4\pi}} Z\begin{vmatrix} 0 \\ \mathbf{k}_\parallel \end{vmatrix}(\chi, 1), \tag{129}$$

where we have used equation (B.5) and (equation (C.2)) that $C \to 0$ as $\sigma \to 0$ in 3D. In equation (128) for $d_\Lambda = 2$, χ is a positive quadratic form defined by the scalar product of the basis vector of Λ, $\chi_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$. (For $d_\Lambda = 1$, all the quadratic forms χ reduce to an absolute value.) The Epstein zeta function in equation (128) converges absolutely for Re $\nu > d_\Lambda$ and can be analytically continued to an entire function in the complex variable ν unless $\mathbf{k}_\parallel \in \Lambda^*$, in which case the Epstein zeta function possesses a simple pole for $\nu = d_\Lambda$.

Interestingly enough, for $d_\Lambda = 2, d = 3, \nu = 1$, the Epstein zeta function can be expressed in a closed form in terms of Jacobi theta functions [14]. For a 1D periodicity in 3D with a period a one then, starting from equation (44), obtains in the limit $\sigma \to 0$

$$D_{00}(0, \mathbf{k}_\parallel) = \frac{1}{\sqrt{4\pi}a} \ln[2 - 2\cos(\mathbf{k}_\parallel a)]. \tag{130}$$

The expression is obviously singular for $\mathbf{k}_\parallel \in \Lambda^*$, in accordance with the singularity of the Epstein zeta function for $\nu = d_\Lambda = 1$.

Regarding the Epstein zeta functions, note that one could have written dual representations in the limit $\sigma \to 0$ for $R_\perp = 0, d = 3$, and provided that $\mathbf{k}_\parallel \notin \Lambda^*$, as

$$G_{0\Lambda}(\sigma, \mathbf{k}_\parallel, \mathbf{R}) = -\frac{e^{i\mathbf{k}_\parallel \cdot \mathbf{R}_\parallel}}{2v_0} Z \begin{vmatrix} \mathbf{k}_\parallel \\ \mathbf{R}_\parallel \end{vmatrix} (\chi, 1), \tag{131}$$

where

$$Z \begin{vmatrix} \mathbf{k}_\parallel \\ \mathbf{R}_\parallel \end{vmatrix} (\chi, \nu) = \sum_{\mathbf{k}_n \in \Lambda^*}{}' \frac{e^{i\mathbf{k}_n \cdot \mathbf{R}_\parallel}}{|\mathbf{k}_\parallel + \mathbf{k}_n|^\nu}. \tag{132}$$

7. Discussion

7.1. The choice of the Ewald parameter η

Each of the exponentially convergent Ewald representations (38), (40), (41) for $G_{0\Lambda}$ can be viewed as a one-parametric family of representations. A corresponding image-like series (3) and a dual representation (equations (21), (23)) can be seen then as two ends of the one-parametric continuous spectrum of the representations for $G_{0\Lambda}$. Obviously, by varying the point η, at which the integration is split, the convergence characteristics of the representation can be altered. In most cases, the value of the Ewald parameter η is chosen to balance the convergence of respective $D_L^{(1)}$ and $D_L^{(2)}$ contributions. This leads occasionally to the criticism that an arbitrary optimization parameter enters the evaluation of lattice sums. In contrast, the invariance of D_L's on the value of Ewald parameter η serves as a check of a correct numerical implementation. The Ewald parameter η can often be varied by several orders of magnitude without affecting the results in a wide frequency window. However, for some range of η values one can enter a numerically unstable region: the respective $D_L^{(1)}$ and $D_L^{(2)}$ contributions have opposite signs and similar magnitude, which is several orders larger than the magnitude of resultant D_L. This instability can easily be remedied by the choice of some other value of η, or one can follow the recipe of Berry [24] and chose η to depend on σ and l, and thereby prevent numerical instability completely. Indeed, although the results presented here have been obtained by a uniform l-independent choice of η, one can easily modify the above derivations to the case of l-dependent η [24].

7.2. Numerical convergence

Exponentially convergent representations of lattice sums summarized here provide a significant advantage in terms of computational speed, while maintaining accuracy, over alternative expressions of lattice sums. In the special case of a 1D periodicity in 2D this is demonstrated in table 1. In the case of 1D periodicity in 2D, even with the latest progress due to Yasumoto

Table 1. Quasi-periodic Green's function $G_{0\Lambda}$ for off-axis incidence at an angle $\theta = \pi/8$ upon a 1D lattice oriented along the x-axis in 2D with $\lambda/v_0 = 0.23$. Here, v_0 is the length of a period (primitive lattice cell) along the x-axis. In rows labelled by D, values of $G_{0\Lambda}$ are obtained by a direct summation of its dual representation (spectral-domain form) (taken from table 3 of [33]). These data are compared against those in rows labelled by E, obtained by the (complete) Ewald–Kambe summation (equations (86), (103), (119) with the Ewald parameter $\eta = 0.011$). Data in the respective rows labelled by YY and NMcP are those obtained by Yasumoto and Yoshitomi [35] and Nicorovici and McPhedran [33] methods.

	x	y	Re $G_{0\Lambda}$	Im $G_{0\Lambda}$
D	0.2	0.03	0.117 120 006 144 932	−0.108 131 857 633 201
E			0.117 120 006 144 932	−0.108 131 857 633 206
YY			0.117 120 006 144 941	−0.108 131 857 633 206
NMcP			0.117 120 006 141 860	−0.108 131 857 633 197
D	0.2	0.003	0.115 891 895 634 567	−0.103 497 063 599 642
E			0.115 891 895 634 565	−0.103 497 063 599 651
YY			0.115 891 895 634 577	−0.103 497 063 599 646
NMcP			0.115 891 895 630 095	−0.103 497 063 599 643
D	0.2	0.0003	0.115 881 138 140 449	−0.103 450 147 416 784
E			0.115 881 138 140 448	−0.103 450 147 416 794
YY			0.115 881 138 140 457	−0.103 450 147 416 788
NMcP			0.115 881 138 135 960	−0.103 450 147 416 785

and Yoshitomi [35], it took 40 s to compute $G_{0\Lambda}$ on SPARC workstation from lattice sums with 14 digits accuracy at a single point and frequency. This was in striking contrast to the calculation of exponentially convergent lattice sums in the so-called bulk cases, i.e., when $G_{0\Lambda}$ is periodic in all space dimensions. The lattice sums for an infinite 2D lattice in 2D [23] and an infinite 3D lattice in 3D [2]. The respective convergence times (on a PC with Pentium II processor) for a set of bulk 2D and 3D lattice sums with six digits accuracy are less than $\approx$0.03 s (for a cut-off value of $l_{\max} = 20$) [61] and $\approx$0.8 s (for a cut-off value of $l_{\max} = 6$) [60].

The computational time to reproduce a value of $G_{0\Lambda}$ in table 1 with accuracy of within 8×10^{-15} of that obtained by a direct summation turns out to be $\approx$0.2 s, in line with the respective $\approx$0.03 s and $\approx$0.8 s for convergence time of a set of bulk 2D [61] and 3D lattice sums [60] with six digits accuracy. This should be compared to 1232 s of Nicorovici and McPhedran [33] or to 40 of Yasumoto and Yoshitomi [35] (the computational times have been taken from [35]). The exponentially convergent representation (equations (86), (103), (119)) (i) can be implemented numerically more simply and (ii) converges roughly 200 times faster than the previous best representation [35]. Of the cases tested, the simplest case of a constant $\eta = 0.011$ was chosen.

For a 2D periodicity in 3D, a comparison of the speed and accuracy of exponentially convergent representation of lattice sums (equations (85), (102), (118)) with respect to alternative expressions for $G_{0\Lambda}$ has been summarized in [27]. Again, exponentially convergent representation of lattice sums turns out to be convergent for a given accuracy significantly faster.

The reader is invited to perform some additional tests by using several publicly available F77 codes. In the case of a 2D periodicity in 3D, numerical codes can be obtained from *Comput. Phys. Commun.*: for a complex 2D lattice in 3D see routines DLMNEW and DLMSET of [66], for a simple 2D Bravais lattice in 3D see routine XMAT of [71]. The above codes have been implemented in electronic, acoustic and electromagnetic LKKR codes and successfully tested time and again in various cases [22, 64–67, 69, 71, 72]. A limited Windows executable which incorporates the lattice sums within a photonic LKKR code for the calculation of reflection, transmission and absorption of an electromagnetic plane wave incident on a square array of finite length cylinders arranged on a homogeneous slab of finite thickness is available following the link http://www.wave-scattering.com/caxsrefl.exe.

F77 source code for a 1D Bravais periodicity in 2D is freely available at http://www.wave-scattering.com/ola.f (implementation instruction are described on http://www.wave-scattering.com/dlsum1in2.html). The code has been implemented in a corresponding LKKR code and successfully tested against experiment in [73]. A limited Windows executable calculating the reflection, transmission and absorption of an electromagnetic plane wave incident on a square array of infinite length cylinders in the plane normal to the cylinder axis is available following the link http://www.wave-scattering.com/rta1in2k.exe.

7.3. Outlook

The present work can be straightforwardly extended in several directions. First, as in bulk cases [1, 2], for a 2D periodicity in 3D [4], and for a 1D periodicity in 2D [5], the condition of a simple lattice for a 1D periodicity in 3D can easily be relaxed to an arbitrary periodic lattice. Note that the case of a non-Bravais lattice additionally requires the calculation of the series (1) with the origin of coordinates displaced from the lattice by a fixed nonzero vector. Consequently, the term involving $r_n = 0$ is no longer singular. Therefore, in the latter case the lattice sums are expressed as the sum of solely $D_L^{(1)}$ and $D_L^{(2)}$, where $D_L^{(2)}$ does include the $r_n = 0$ term. These supplementary series can easily be determined following the recipes of [1–4].

Second, following the work of Ohtaka [67] and Modinos [68] for a 2D periodicity in 3D, in the vector case of electromagnetic waves for a 1D periodicity in 3D, the lattice sums and structure constants can easily be obtained from those in the scalar case presented here (2D case is trivial as it reduces to a scalar problem). It is only required to multiply the scalar quantities with appropriate numerical factors of geometric origin [58, 59, 67, 68]. This possibility is a consequence of a fact, as first shown by Stein [80], that vector translational addition coefficients can be derived from pertinent scalar addition coefficients. A more involved, but possible, is a generalization of the presented results to semi-infinite cases, when periodicity is imposed on a half-line or in a half-space only [34, 37, 81].

8. Summary and conclusions

A classical problem of free-space Green's functions $G_{0\Lambda}$ representations of the Helmholtz equation was studied in various quasi-periodic cases, i.e., when an underlying periodicity is imposed in less dimensions than is the dimension of an embedding space. Exponentially convergent series for the free-space quasi-periodic $G_{0\Lambda}$ and for the expansion coefficients D_L of $G_{0\Lambda}$ in the basis of regular (cylindrical in two dimensions and spherical in three dimension (3D)) waves, or lattice sums, were reviewed and new results for the case of a one-dimensional (1D) periodicity in 3D were derived. The derivation of relevant results highlighted the common part which is applicable to any of the quasi-periodic cases.

Exponentially convergent Ewald representations (38), (40), (41) for $G_{0\Lambda}$ (see also section 6.2) and for lattice sums D_L hold for any value of the Bloch momentum and allow $G_{0\Lambda}$ to be efficiently evaluated also in the periodicity plane. After substituting the resulting expressions for $D_L^{(1)}$ (equations (83), (85), (86)), $D_L^{(2)}$ (equations (102), (103)) and $D_L^{(3)}$ (equations (118), (118), (119)) into defining equation (46) for D_L, an alternative exponentially

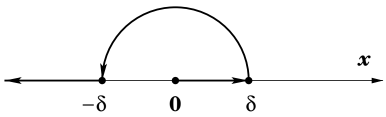

Figure 3. Integration contour in the Schläfli integral representation of $H_\nu^{(1)}$.

convergent representation for Schlömilch series (11) of cylindrical and spherical Hankel functions of any integer order was obtained.

The quasi-periodic Green's functions of the Laplace equation were studied as the limiting case of the corresponding Ewald representations of $G_{0\Lambda}$ of the Helmholtz equation by taking the limit of the wave vector magnitude going to zero. Thereby, exponentially convergent representations of $G_{0\Lambda}$ in the Laplace case were obtained, which are convergent (unless $\mathbf{R} \in \Lambda$) also in the periodicity plane. An alternative exponentially convergent series for $G_{0\Lambda}$ for 1D periodicity in 3D in the Laplace case has also been obtained earlier by Linton (see series in equation (3.26) of [30]). However, our expressions have been derived without any artificial regularization using a convergence ensuring logarithmically divergent series (cf [30]).

The results obtained can be useful for numerical solution of boundary integral equations for potential flows in fluid mechanics, remote sensing of periodic surfaces, periodic gratings, in many contexts of simulating systems of charged particles, in molecular dynamics, for solving the spectrum of particular open resonators, for the description of quasi-periodic arrays of point interactions in quantum mechanics, linear chains of spheres and nanoparticles in optics and electromagnetics, and of infinite arrays of resonators coupled to a waveguide, and in various *ab initio* first-principle multiple-scattering theories for the analysis of diffraction of classical and quantum waves.

Appendix A. Integral representations of $H_\nu^{(1)}$

For the Ewald summation with $\mathbf{r}_s = 0$ excluded, one uses the Schläfli integral representation,

$$H_\nu^{(1)}(z) = \frac{1}{\pi \mathrm{i}} \int_{C_-} u^{-\nu-1}\, \mathrm{e}^{\frac{1}{2}z\left(u-\frac{1}{u}\right)}\, \mathrm{d}u, \tag{A.1}$$

where the contour C_- is the contour which goes from the origin to $\delta > 0$, continues along a semicircle in the upper half-plane with radius δ to $-\delta$, and goes along the negative real axis to infinity (see figure 3). This results in an exponentially decreasing integrand at the integration contour ends for $\operatorname{Re} z > 0$. The Schläfli representation, which yields the Hankel functions $H_\nu^{(1)}(z)$ as moments of the generating function of the Bessel functions $J_l(z)$ (see [7], p 14), is obtained upon substitution $u = e^t$ in the integral representation (see (9.1.25) of [16]),

$$H_\nu^{(1)}(z) = \frac{1}{\pi \mathrm{i}} \int_{-\infty}^{\infty+\pi \mathrm{i}} \mathrm{e}^{z \sinh t - \nu t}\, \mathrm{d}t, \tag{A.2}$$

which is valid for $|\arg z| < \pi/2$.

Setting in the Schläfli representation (A.1) $z = \sigma r$ and

$$t = -\frac{2r}{\sigma}\xi^2, \qquad \mathrm{d}u = -2\left(\frac{\sigma}{2r}\right)^{-1} \xi\, \mathrm{d}\xi, \tag{A.3}$$

one arrives at

$$H_\nu^{(1)}(\sigma r) = \frac{2i^{-2\nu-1}}{\pi} \left(\frac{\sigma}{2r}\right)^{\nu} \int_C \xi^{-2\nu-1}\, \mathrm{e}^{-r^2\xi^2+\sigma^2/(4\xi^2)}\, \mathrm{d}\xi, \tag{A.4}$$

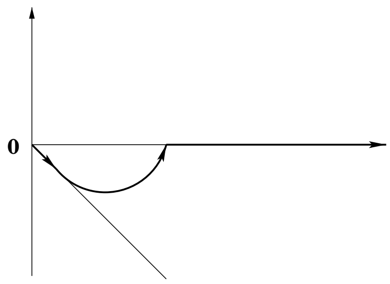

Figure 4. Integration contour in the Ewald integral representation of $H_\nu^{(1)}$.

where C is the so-called Ewald contour (see figure 4), which leaves the origin along the ray $\arg \xi = \arg \sigma - \pi/4$, then returns to the real axis and continues along the positive real axis to infinity.

Upon substituting in the Schläfli representation (A.1) $z = \sigma r$ and

$$u = \frac{r}{\sigma}\zeta, \tag{A.5}$$

one arrives at

$$H_\nu^{(1)}(\sigma r) = \frac{1}{\pi \mathrm{i}} \left(\frac{\sigma}{r}\right)^\nu \int_C \zeta^{-\nu-1}\, \mathrm{e}^{\frac{1}{2}(r^2\zeta - \sigma^2/\zeta)}\, \mathrm{d}\zeta. \tag{A.6}$$

Let us consider for a while σ as a general real parameter. Then, following discussion at the end of appendix 2 of [21], the Schläfli integration contour for a positive σ^2 can be deformed to that shown in figure 2. Afterward, with the use of Jordan's lemma ([48], p 115) integration contour can be deformed to that from 0 to $\mathrm{i}\infty$ on the imaginary axis. For a negative σ^2 one would then, as a result of the substitution (A.5), arrive at the contour from 0 to ∞ along the positive real axis (see appendix 2 of [21]).

Eventually, we provide Hobson's representation for the modified Bessel functions of the third kind [11]:

$$\left(\frac{q}{k}\right)^\nu K_\nu(kq) = \int_0^\infty \zeta^{\nu-1}\, \mathrm{e}^{-\frac{1}{2}(k^2\zeta + q^2/\zeta)}\, \mathrm{d}\zeta. \tag{A.7}$$

Appendix B. Properties of harmonics $\mathcal{Y}_L$

Throughout this paper complex harmonics $\mathcal{Y}_L$ (cylindrical, $Y_l = \mathrm{e}^{\mathrm{i}l\phi}/\sqrt{2\pi}$, for $d = 2$ and spherical for $d = 3$ [4, 16, 22, 65]; for 1D harmonics see [49]) are used. Under complex conjugation, they behave according to

$$\mathcal{Y}_L^*(\hat{\mathbf{R}}) = \begin{cases} \mathcal{Y}_l(\hat{\mathbf{R}}), & \text{1D}, \\ \mathcal{Y}_{-l}(\hat{\mathbf{R}}), & \text{2D}, \\ (-1)^m \mathcal{Y}_{l-m}(\hat{\mathbf{R}}), & \text{3D}. \end{cases} \tag{B.1}$$

In 3D the property goes under the name of the Condon–Shortley convention. In any dimension, the harmonics satisfy the inversion formula

$$\mathcal{Y}_L(-\hat{\mathbf{r}}) = (-1)^l \mathcal{Y}_L(\hat{\mathbf{r}}), \tag{B.2}$$

the orthonormality

$$\oint \mathcal{Y}_L(\hat{\mathbf{r}}) \mathcal{Y}_{L'}^*(\hat{\mathbf{r}})\, \mathrm{d}\Omega = \delta_{LL'} \tag{B.3}$$

and closure

$$\sum_L \mathcal{Y}_L(\hat{\mathbf{r}})\mathcal{Y}_L^*(\hat{\mathbf{r}}') = \delta_\Omega(\mathbf{r}, \mathbf{r}'). \tag{B.4}$$

Here, $\delta_\Omega(\mathbf{r}, \mathbf{r}')$ is the delta function on the unit sphere whereas $\mathrm{d}\Omega$ is the usual angular measure which is determined by the relation $\mathrm{d}\mathbf{r} = r^{d-1}\,\mathrm{d}r\,\mathrm{d}\Omega$. (In 1D the angular integral $\oint \mathrm{d}\Omega$ reduces to the summation over the forward and backward directions.)

Note that in any dimension,

$$\mathcal{Y}_0 = \frac{1}{\sqrt{A}}. \tag{B.5}$$

Since $\mathcal{Y}_0$ is a constant, combining equation (B.5) with the orthonormality (B.3) of $\mathcal{Y}_L$ yields

$$\oint \mathcal{Y}_L(\hat{\mathbf{r}})\,\mathrm{d}\Omega = \sqrt{A}\delta_{L0}. \tag{B.6}$$

B.1. The plane-wave expansion

An expansion of the plane-wave expansion in the angular momentum basis is

$$\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} = A\sum_L \mathrm{i}^{|l|}\mathcal{J}_{|l|}(kr)\mathcal{Y}_L(\hat{\mathbf{r}})\mathcal{Y}_L^*(\hat{\mathbf{k}}) = A\sum_L \mathrm{i}^{|l|}\mathcal{J}_{|l|}(kr)\mathcal{Y}_L^*(\hat{\mathbf{r}})\mathcal{Y}_L(\hat{\mathbf{k}}), \tag{B.7}$$

where

$$A = \oint \mathrm{d}\Omega = \begin{cases} 2, & \text{1D}, \\ 2\pi, & \text{2D}, \\ 4\pi, & \text{3D}, \end{cases} \tag{B.8}$$

where $\mathrm{d}\Omega$ is the usual angular measure. The series (B.7) converges uniformly as $|\mathbf{k}|$ and $\mathbf{r}$ run through compact sets of $\mathbb{R}$ and $\mathbb{R}^3$ (theorem XI.64f of [79]). The absolute value of l is used in (B.7) in case the sum over angular momenta in 2D runs from minus to plus infinity.

The plane-wave expansion (B.7) is also valid for complex arguments. It is interesting to note that $\mathcal{Y}_L^*$ is no longer the complex conjugate of $\mathcal{Y}_L$ for complex $\mathbf{k}$ (e.g., in 3D because of the complex nature of associated Legendre functions). However, the relations (B.1) remain the same as in the case of harmonics of a real argument [4, 65]. For 3D case see, for instance, appendix 1 of [4] or appendix A of review by Tong [65]. The 2D case follows by a straightforward adaptation of the 3D case, whereas the 1D case is trivial [49].

Appendix C. Free-space scattering Green's function

One has (see equation (5))

$$G_0^+(\sigma, \mathbf{r}, \mathbf{r}') = \frac{1}{(2\pi)^d}\int \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{\sigma^2 - k^2 + \mathrm{i}\epsilon}d^d\mathbf{k} = -\mathrm{i}C\mathcal{H}_0^+(\sigma|\mathbf{r}-\mathbf{r}'|), \tag{C.1}$$

where

$$C = \frac{\pi}{2}\frac{A}{(2\pi)^d}\sigma^{d-2} = \begin{cases} \frac{1}{2\sigma}, & \text{1D}, \\ \frac{1}{4}, & \text{2D}, \\ \frac{\sigma}{4\pi}, & \text{3D}, \end{cases} \tag{C.2}$$

is a real positive number for positive energies. The second equality in (5) is established by expanding the exponential into regular waves according to equation (B.7), performing the angular integral using the identity (B.6) satisfied by the harmonics $\mathcal{Y}_L$, and eventually performing the remaining radial integral using the integral identity

$$I = \int_0^\infty \frac{\mathcal{J}_0(kr)}{\sigma^2 + \mathrm{i}\epsilon - k^2} k^{d-1}\, dk = -\frac{\pi\,\mathrm{i}}{2}\sigma^{d-2}\mathcal{H}_0^+(\sigma r), \tag{C.3}$$

which can be easily established by contour integration in complex plane. On arriving at equation (C.3), one substitutes for J_0 according to

$$\mathcal{J}_l(kr) = \tfrac{1}{2}\left[\mathcal{H}_l^+(kr) + \mathcal{H}_l^-(kr)\right] \tag{C.4}$$

and applies the identity (analyticity property)

$$\mathcal{H}_l^-(z\,\mathrm{e}^{-\pi\mathrm{i}}) = (-1)^{l+d+1}\mathcal{H}_l^+(z) \tag{C.5}$$

(see equations (9.1.16) and (10.1.18) of [16] and [49]) for $l = 0$.

One can show that

$$|\mathbf{x} - \mathbf{y}| \sim |\mathbf{x}| - \frac{\mathbf{x}\cdot\mathbf{y}}{|\mathbf{x}|} + \mathcal{O}(1/|\mathbf{x}|^2) \qquad \text{as} \quad |\mathbf{x}| \to \infty. \tag{C.6}$$

Therefore, upon using the asymptotic properties (2) of $\mathcal{H}_0^+(\sigma|\mathbf{x}-\mathbf{y}|)$ for $|\mathbf{x}| \to \infty$,

$$G_0^+(\mathbf{x},\mathbf{y}) \sim f_\sigma(|\mathbf{x}|)\,\mathrm{e}^{-\mathrm{i}\sigma\mathbf{x}\cdot\mathbf{y}/|\mathbf{x}|} = f_\sigma(|\mathbf{x}|)\,\mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{y}}, \tag{C.7}$$

where

$$f_\sigma(|\mathbf{x}|) \sim G_0^+(\mathbf{x},\mathbf{0})|_{\mathbf{x}\to\infty} = -\mathrm{i}C\mathcal{H}_0^+(\sigma|\mathbf{x}|), \qquad \mathbf{k}' = \sigma\mathbf{x}/|\mathbf{x}|. \tag{C.8}$$

Function $f_\sigma(|\mathbf{x}|)$ describes outgoing waves in a given dimension. Explicitly,

$$f_\sigma(|\mathbf{x}|) = \begin{cases} -\frac{\mathrm{i}}{2\sigma}\,\mathrm{e}^{\mathrm{i}\sigma|\mathbf{x}|}, & \text{1D}, \\ -\frac{\mathrm{i}}{\sqrt{8\pi\sigma}}\frac{\mathrm{e}^{\mathrm{i}\sigma|\mathbf{x}|-\mathrm{i}\pi/4}}{\sqrt{|\mathbf{x}|}}, & \text{2D}, \\ -\frac{1}{4\pi}\frac{\mathrm{e}^{\mathrm{i}\sigma|\mathbf{x}|}}{|\mathbf{x}|}, & \text{3D}. \end{cases} \tag{C.9}$$

The product AC in the partial wave expansion (9) of the free Green's function can be independently determined from the condition that the discontinuity of radial derivatives of the free Green's function at coinciding arguments multiplied by r^{d-1} is exactly 1. The factor r^{d-1} follows from a fact that the integral measure $\mathrm{d}\mathbf{r}$ can be written as $\mathrm{d}\mathbf{r} = r^{d-1}\,\mathrm{d}r\,\mathrm{d}\Omega$. Since the harmonics $\mathcal{Y}_L$ are orthonormal in the measure $\mathrm{d}\Omega$ (equation (B.3)), the discontinuity of radial derivatives of the free Green's function in the absence of any prefactor in (9) can be conveniently expressed by the Wronskian

$$W_r[\mathcal{J}_l(\sigma r), \mathcal{H}_l^+(\sigma r)] = i\,W_r[\mathcal{J}_l(\sigma r), \mathcal{N}_l(\sigma r)] \tag{C.10}$$

where

$$W_x[f(ax), g(ax)] = f(ax)g'(ax) - f'(ax)g(ax),$$

and prime denotes first derivative with respect to x. Now

$$W_r[\mathcal{J}_l(\sigma r), \mathcal{N}_l(\sigma r)] = \sigma\,W_z[\mathcal{J}_l(z), \mathcal{N}_l(z)]$$

where $z = \sigma r$.

Knowing the Wronskian

$$W_z[\mathcal{J}_l(z), \mathcal{N}_l(z)] = \mathcal{J}_l\mathcal{N}_l' - \mathcal{J}_l'\mathcal{N}_l = \begin{cases} 1, & \text{1D}, \\ 2/(\pi z), & \text{2D}, \\ 1/z^2, & \text{3D}, \end{cases} \tag{C.11}$$

the product AC can be then found directly from the discontinuity given by the relation

$$AC = \{\sigma r^{d-1} W_z[\mathcal{J}_l(z), \mathcal{N}_l(z)]\}^{-1}. \tag{C.12}$$

Appendix D. Jacobi identities

The equivalence of the lattice sum (see equation (3)) and the eigenvalue expansion (see equation (13)) in the case of the heat equation with the Bloch boundary conditions in a box leads to the identity

$$K_\Lambda(\mathbf{R},t) = \frac{1}{(4\pi t)^{d/2}} \sum_{\mathbf{r}_s\in\Lambda} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_s}\, \mathrm{e}^{-(\mathbf{R}-\mathbf{r}_s)^2/(4t)} = \frac{1}{v_0} \sum_{\mathbf{k}_n\in\Lambda^*} \mathrm{e}^{-(\mathbf{k}+\mathbf{k}_n)^2 t}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}+\mathbf{k}_n)\cdot\mathbf{R}}. \tag{D.1}$$

In a special case, for a simple cubic lattice with a unit lattice constant one has $\Lambda = \Lambda^*$. Upon substituting $\mathbf{k}_n = 2\pi\mathbf{n}$, with $\mathbf{n}$ being an integer valued vector, and $\mathbf{R} = \mathbf{k} = 0$, identity (D.1) yields

$$\frac{1}{(4\pi t)^{d/2}} \sum_{\mathbf{n}\in\Lambda} \mathrm{e}^{-\mathbf{n}^2/(4t)} = \sum_{\mathbf{n}\in\Lambda} \mathrm{e}^{-4\pi^2\mathbf{n}^2 t}. \tag{D.2}$$

For $d = 1$, the latter is a special $\theta = 0$ case of the famous number theoretical Jacobi theta function identity (upon rescaling $t \to 4\pi t$),

$$\sum_{n=-\infty}^{\infty} \exp(-\pi n^2 t - 2\pi \mathrm{i} n\theta) = t^{-1/2} \sum_{l=-\infty}^{\infty} \exp[-\pi(l+\theta)^2/t], \tag{D.3}$$

which is valid for a complex θ and $\mathrm{Re}\, t > 0$. The Jacobi theta function identity can also be proved by applying the Poisson sum rule and is also sometimes referred to as Poisson–Jacobi formula.

An alternative form (35) of the Jacobi formula, as has been used by Kambe [4, 20, 21], is obtained upon substitution $t = \zeta/2$ and is valid for $\mathrm{Re}\,\zeta > 0$. After the substitution $t = 1/(4\xi^2)$, the generalized Jacobi identity (D.1) yields

$$\sum_{\mathbf{r}_s\in\Lambda} \mathrm{e}^{-(\mathbf{R}-\mathbf{r}_s)^2\xi^2 + \mathrm{i}\mathbf{k}\cdot\mathbf{r}_s} = \frac{\pi^{d/2}}{v_0\xi^d} \sum_{\mathbf{k}_n\in\Lambda^*} \mathrm{e}^{-(\mathbf{k}_n+\mathbf{k})^2/(4\xi^2) + \mathrm{i}(\mathbf{k}+\mathbf{k}_n)\cdot\mathbf{R}}. \tag{D.4}$$

In like manner, upon the substitution $\mathbf{R} \to -\mathbf{R}$, $\mathbf{k} \to -\mathbf{k}$, $\mathbf{k}_n \to -\mathbf{k}_n$, one finds

$$\sum_{\mathbf{r}_s\in\Lambda} \mathrm{e}^{-(\mathbf{R}+\mathbf{r}_s)^2\xi^2 - \mathrm{i}\mathbf{k}\cdot(\mathbf{R}+\mathbf{r}_s)} = \frac{\pi^{d/2}}{v_0\xi^d} \sum_{\mathbf{k}_n\in\Lambda^*} \mathrm{e}^{-(\mathbf{k}_n+\mathbf{k})^2/(4\xi^2) + \mathrm{i}\mathbf{k}_n\cdot\mathbf{R}}. \tag{D.5}$$

The last two identities are often referred to as the Ewald identities (cf [2, 18, 19]).

Appendix E. General properties of free-space quasi-periodic Green's functions and of lattice sums

For any $\mathbf{r}_s \in \Lambda$, $\mathbf{k}_n \in \Lambda^*$, $G_{0\Lambda}$ satisfies the following trivial properties:

$$G_{0\Lambda}(\sigma,\mathbf{k}_\parallel,\mathbf{R}) = G_{0\Lambda}(\sigma,\mathbf{k}_\parallel,\mathbf{R}+\mathbf{r}_s) = G_{0\Lambda}(\sigma,\mathbf{k}_\parallel+\mathbf{k}_n,\mathbf{R}). \tag{E.1}$$

Obviously, $G_{0\Lambda}$ is only a function of the projection $\mathbf{k}_\parallel$ of $\mathbf{k}$ upon Λ^* (note that $\mathbf{k}_\parallel = \mathbf{k}$ for $d_\Lambda = d$).

Except for the frequencies which satisfy $\sigma^2 = (\mathbf{k}_\parallel + \mathbf{k}_n)^2$ for some $\mathbf{k}_n \in \Lambda^*$, $G_{0\Lambda}$ satisfies the following *reflection symmetry* property [20, 21]:

$$G_{0\Lambda}(\sigma,\mathbf{k}_\parallel,\mathbf{R}_\parallel+\mathbf{R}_\perp) = G_{0\Lambda}(\sigma,\mathbf{k}_\parallel,\mathbf{R}_\parallel-\mathbf{R}_\perp). \tag{E.2}$$

From dual representations (21), (23) it follows that the respective $G_{0\Lambda}$ are *Hermitian* for the interchange of variables $\mathbf{r}_\parallel$ and $\mathbf{r}'_\parallel$ and *complex symmetric* for the interchange of variables $r_\perp$ and $r'_\perp$.

Obviously, for any $\mathbf{r}_n \in \Lambda$ also $-\mathbf{r}_n \in \Lambda$. Upon combining the inversion formula (B.2) of angular-momentum harmonics $\mathcal{Y}_L$ with the defining equation (11) for D_L one finds

$$D_L(\sigma, \mathbf{k}_\parallel) = -\mathrm{i}CA^{1/2}\delta_{L0} - \mathrm{i}AC \sum_{\mathbf{r}_n \in \bar{\Lambda}} {}'\mathcal{H}_l^+(\sigma r_n)\mathcal{Y}_L^*(\hat{\mathbf{r}}_n) \begin{cases} 2\cos(\mathbf{k}_\parallel \cdot \mathbf{r}_n), & l \text{ even} \\ 2\mathrm{i}\sin(\mathbf{k}_\parallel \cdot \mathbf{r}_n), & l \text{ odd.} \end{cases} \tag{E.3}$$

The summation here is performed over the subset $\bar{\Lambda} \subset \Lambda$ of equivalence classes of $\mathbf{r}_n \in \Lambda$ with respect to spatial inversion $\mathbf{r}_n \to -\mathbf{r}_n$. Thus, for l *even* the corresponding lattice sums $D_L(\sigma, \mathbf{k}_\parallel)$ are *even* functions of the Bloch vector $\mathbf{k}_\parallel$,

$$D_L(\sigma, \mathbf{k}_\parallel) = D_L(\sigma, -\mathbf{k}_\parallel). \tag{E.4}$$

In the special case of a 2D periodicity in 3D one has additionally

$$D_L(\sigma, \mathbf{k}_\parallel) = D_L\left(\sigma, \mathbf{k}_\parallel^\pm\right) = D_L\left(\sigma, \mathbf{k}_\parallel^\mp\right), \tag{E.5}$$

where the respective wave vectors $\mathbf{k}_\parallel^\pm = (k_1, -k_2)$, $\mathbf{k}_\parallel^\mp = (-k_1, k_2)$ are formed from the Bloch vector $\mathbf{k}_\parallel$ components k_1 and k_2.

In the special case of $D_{00}(\sigma, \mathbf{k}_\parallel)$ for $\sigma = \mathrm{i}\sqrt{-z}$, there are known some further general analytic properties in the complex z-plane, which have been established by Karpeshina [13, 47]:

- $D_{00}(\mathrm{i}\sqrt{-z}, \mathbf{k}_\parallel)$ is for a fixed Bloch vector $\mathbf{k}_\parallel$ an analytic function on the complex plane cut along the real half-axis $z > |\mathbf{k}_\parallel|^2$ with $\mathrm{Im}\, D_{00} \neq 0$ on both sides of the cut.
- On the real half-axis $z < |\mathbf{k}_\parallel|^2$, the function $D_{00}(\mathrm{i}\sqrt{-z}, \mathbf{k}_\parallel)$ is real, smooth and increases monotonically $(0 < \partial_z D_{00}(\mathrm{i}\sqrt{-z}, \mathbf{k}_\parallel) < \infty)$ from $-\infty$ to ∞.

Appendix F. Alternative definitions of lattice sums and structure constants

If instead of D_Λ of equation (7) the difference

$$\mathcal{D}_\Lambda(\sigma, \mathbf{k}_\parallel, \mathbf{R}) = G_{0\Lambda}(\sigma, \mathbf{k}, \mathbf{R}) - G_0(\sigma, \mathbf{R}), \tag{F.1}$$

which is also regular for $\mathbf{R} \to 0$, is expanded in terms of the regular waves,

$$\mathcal{D}_\Lambda(\sigma, \mathbf{k}_\parallel, \mathbf{R}) = \sum_L \mathcal{D}_L(\sigma, \mathbf{k}_\parallel)\mathcal{J}_l(\sigma R)\mathcal{Y}_L(\hat{\mathbf{R}}) \tag{F.2}$$

$$= \sum_{L,L'} g_{LL'}(\sigma, \mathbf{k}_\parallel)\mathcal{J}_l(\sigma r)\mathcal{J}_{l'}(\sigma r')\mathcal{Y}_L(\hat{\mathbf{r}})\mathcal{Y}_{L'}^*(\hat{\mathbf{r}}'), \tag{F.3}$$

this results in alternative lattice sums $\mathcal{D}_L$ and structure constants $g_{LL'}$. We recall here that the structure constants can in a known way be unambiguously determined from the lattice sums [53].

The lattice sums $\mathcal{D}_L$ and D_L and structure constants $A_{LL'}$ and $g_{LL'}$, where

$$D_\Lambda(\sigma, \mathbf{k}_\parallel, \mathbf{R}) = \sum_{L,L'} A_{LL'}(\sigma, \mathbf{k}_\parallel)\mathcal{J}_l(\sigma r)\mathcal{J}_{l'}(\sigma r')\mathcal{Y}_L(\hat{\mathbf{r}})\mathcal{Y}_{L'}^*(\hat{\mathbf{r}}'), \tag{F.4}$$

are related to each other as follows:

$$\mathcal{D}_L(\sigma, \mathbf{k}_\parallel) = D_L(\sigma, \mathbf{k}_\parallel) + \mathrm{i}CA^{1/2}\delta_{L0}, \tag{F.5}$$

$$g_{LL'}(\sigma, \mathbf{k}_\parallel) = A_{LL'}(\sigma, \mathbf{k}_\parallel) + \mathrm{i}AC\delta_{LL'}. \tag{F.6}$$

A and C here are the familiar numerical constants which have been defined by equations (B.8) and (C.2), respectively. Relations (F.5) and (F.6) follow easily from

$$\begin{aligned} \mathrm{i}\,\mathrm{Im}\, G_0^+(\sigma, \mathbf{R}) &= -\mathrm{i}C\mathcal{J}_0(\sigma R) = -\mathrm{i}CA^{1/2}\mathcal{J}_0(\sigma R)\mathcal{Y}_0(\hat{\mathbf{R}}) \\ &= \sum_{LL'} g^0_{LL'}\mathcal{J}_l(\sigma r)\mathcal{J}_{l'}(\sigma r')\mathcal{Y}_L(\hat{\mathbf{r}})\mathcal{Y}^*_{L'}(\hat{\mathbf{r}}'), \end{aligned} \tag{F.7}$$

where

$$g^0_{LL'} = -\mathrm{i}AC\delta_{LL'}. \tag{F.8}$$

In going from the first to the second equality in (F.7) we have used that in any space dimension $\mathcal{Y}_0(\hat{\mathbf{R}}) = A^{-1/2}$ (equation (B.5)). The final expressions then readily follow from the partial wave expansion of the free Green's function (see equation (9) of appendix C).

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