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Lodder, A.; van Ek, J.

published in

Physical Review B. Condensed Matter
1989

document version

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citation for published version (APA)

Lodder, A., & van Ek, J. (1989). Comment on ``Energy-band equation for a general periodic potential''. *Physical Review B. Condensed Matter*, 40(3), 1979-1980.

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Comment on "Energy-band equation for a general periodic potential"

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(Received 18 July 1988)

The new energy-band equation by Badraxe and Freeman is shown to be an identity.

In this Comment we want to discuss a paper by Badraxe and Freeman¹ concerning the derivation of an energy-band equation for a general periodic potential. It will be shown that what Badraxe and Freeman call their main result [their Eq. (38), denoted Eq. (BF38)], is in fact an identity. In addition, the source of this confusing peculiarity will be revealed.

The partial-wave solution at a given energy E of the Schrödinger equation, pertaining to a system with the crystal potential V^c inside and a zero potential outside a sphere with radius d enclosing a Wigner-Seitz cell Ω , can be written as

$$\phi_L^d(E, \mathbf{r}) = \sum_{L'} [C_{LL'}^d(r) j_{L'}(\mathbf{r}) + S_{LL'}^d(r) n_{L'}(\mathbf{r})], \quad (1)$$

in which

$$C_{LL'}^d(r) = \frac{\pi\sqrt{E}}{2} \int_r^\infty d^3r' n_{L'}^*(\mathbf{r}') V^d(\mathbf{r}') \phi_L^d(E, \mathbf{r}') \quad (2a)$$

and

$$S_{LL'}^d(r) = \frac{\pi\sqrt{E}}{2} \int_0^r d^3r' j_{L'}^*(\mathbf{r}') V^d(\mathbf{r}') \phi_L^d(E, \mathbf{r}'). \quad (2b)$$

The potential V^d is defined by

$$V^d(\mathbf{r}) = \begin{cases} V^c(\mathbf{r}), & \|\mathbf{r}\| \leq d \\ 0, & \text{elsewhere.} \end{cases}$$

These equations arise when the Schrödinger equation in its integral form is broken up in terms referring to specific integration domains [e.g., Eqs. (2.24) and (2.25) of Brown and Ciftan²]. Since the crystal wave function is to be expressed in the set $\{\phi_L^d\}$, these partial waves are bound to be regular at the origin, which implies that

$$C_{LL'}^d(0) = \delta_{LL'}, \text{ and } S_{LL'}^d(0) = 0. \quad (3)$$

In order to prove that $\Gamma(\mathbf{k}, E) \equiv \underline{N}(\mathbf{k}, E) \underline{\Sigma}(\mathbf{k}, E)$ [see Eqs. (BF37) and (BF38)], which reduces, in the $d \rightarrow \infty$ limit, (BF36) to a trivial equation, we first rewrite Eq. (2a) for $r=0$ as follows:

$$\begin{aligned} C_{LL'}^d(0) &= \frac{\pi\sqrt{E}}{2} \int_{(\mathbb{R}^3)} d^3r' n_{L'}^*(\mathbf{r}') V^d(\mathbf{r}') \phi_L^d(E, \mathbf{r}') \\ &= \frac{\pi\sqrt{E}}{2} \int_{(\mathbb{R}^3 \setminus \Omega)} d^3r' n_{L'}^*(\mathbf{r}') V^d(\mathbf{r}') \phi_L^d(E, \mathbf{r}') \\ &\quad + \frac{\pi\sqrt{E}}{2} \int_{(\Omega)} d^3r' n_{L'}^*(\mathbf{r}') V^c(\mathbf{r}') \phi_L^d(E, \mathbf{r}'). \end{aligned} \quad (4)$$

The different integration regions occurring in Eq. (4) and the following are as depicted in Fig. 1.

Combination of the Eqs. (3) and (4) results in the equality

$$\begin{aligned} \frac{\pi\sqrt{E}}{2} \int_{(\mathbb{R}^3 \setminus \Omega)} d^3r' n_{L'}^*(\mathbf{r}') V^d(\mathbf{r}') \phi_L^d(E, \mathbf{r}') \\ = \delta_{LL'} - \frac{\pi\sqrt{E}}{2} \int_{(\Omega)} d^3r' n_{L'}^*(\mathbf{r}') V^c(\mathbf{r}') \phi_L^d(E, \mathbf{r}'). \end{aligned} \quad (5)$$

This equality can be applied directly to (BF37) after the replacement of $\phi_L^d(E, \mathbf{r})$ by the functions $\tilde{\phi}_L^d(\mathbf{k}, E, \mathbf{r})$, which are constructed by a folding procedure [Eq. (BF26)]. So the Γ^d matrix element in (BF37) is equal to

$$\begin{aligned} \Gamma_{LL'}^d(\mathbf{k}, E) &= \frac{\pi\sqrt{E}}{2} \int_{(\mathbb{R}^3 \setminus \Omega)} d^3r' n_{L'}^*(\mathbf{r}') V^d(\mathbf{r}') \\ &\quad \times \tilde{\phi}_L^d(\mathbf{k}, E, \mathbf{r}'). \end{aligned} \quad (6)$$

As stated by Badraxe and Freeman, the functions

$$\tilde{\phi}_L(\mathbf{k}, E, \mathbf{r}) \equiv \lim_{d \rightarrow \infty} \tilde{\phi}_L^d(\mathbf{k}, E, \mathbf{r})$$

possess the Bloch symmetry. In this $d \rightarrow \infty$ limit Eq. (6) can be written as infinite lattice sum:

$$\begin{aligned} \Gamma_{LL'}(\mathbf{k}, E) &\equiv \lim_{d \rightarrow \infty} \Gamma_{LL'}^d(\mathbf{k}, E) \\ &= \sum_{\mathbf{R} (\neq 0)} \frac{\pi\sqrt{E}}{2} \int_{(\Omega)} d^3r' n_{L'}^*(\mathbf{r}' + \mathbf{R}) V^c(\mathbf{r}') \\ &\quad \times e^{i\mathbf{k} \cdot \mathbf{R}} \tilde{\phi}_L(\mathbf{k}, E, \mathbf{r}'). \end{aligned} \quad (7)$$

After the application of the well-known theorem for the expansion of spherical Neumann functions in spherical

FIG. 1. Schematic representation of the different integration regions around the origin, located in the central cell Ω . ($\mathbb{R}^3 \setminus \Omega$) corresponds to all space outside the central cell.

Bessel functions,

$$n_L(\mathbf{r} + \mathbf{R}) = \sum_{L'} N_{LL'}(\mathbf{R}, E) j_{L'}(\mathbf{r}), \quad \|\mathbf{r}\| < \|\mathbf{R}\|$$

and introducing the usual $\mathbf{k}$ -dependent structure matrix,

$$N_{LL'}(\mathbf{k}, E) = \sum_{\mathbf{R} (\neq 0)} N_{LL'}(\mathbf{R}, E) e^{i\mathbf{k} \cdot \mathbf{R}},$$

Eq. (7) is transformed into

$$\begin{aligned} \Gamma_{LL'}(\mathbf{k}, E) &= \sum_{L''} N_{LL''}(\mathbf{k}, E) \frac{\pi \sqrt{E}}{2} \\ &\times \int_{(\Omega)} d^3 r' j_{L''}^*(\mathbf{r}') V^c(\mathbf{r}') \tilde{\phi}_{L'}(\mathbf{k}, E, \mathbf{r}') \\ &= \sum_{L''} N_{LL''}(\mathbf{k}, E) \sum_{L''L'} (\mathbf{k}, E), \end{aligned} \quad (8)$$

which reduces (BF38) to an identity for energies including eigenvalue energies.

This means that, even if one were able to construct functions $\tilde{\phi}_L^d(\mathbf{k}, E, \mathbf{r})$ for large d , the equations presented [(BF36) and (BF38)] are not able to retrieve the quantum label $\mathbf{k}$ for the $A_L(\mathbf{k}, E)$ and the $\psi(n\mathbf{k}, E, \rho)$, (BF23a), remain undetermined. In other words, the basis functions themselves comprise the solution of the problem, albeit in the angular-momentum representation.

We want to stipulate that this tricky situation is inherent to the use of the angular-momentum representation over large regions of the lattice which obscures the translational symmetry of the infinite lattice. In the limit $d \rightarrow \infty$, the functions $\phi_L^d(E, \mathbf{r})$ are the regular solutions at energy E of the Bloch-Schrödinger equation,

$$(E - p^2) \phi_L(E, \mathbf{r}) = V^c(\mathbf{r}) \phi_L(E, \mathbf{r}). \quad (9)$$

If these functions (which in fact are adapted to the crystal potential) are used to construct a manifestly Bloch-symmetric basis (in terms of which the problem will be formulated), one necessarily ends up with a secular equation which gives no new information. This accumulates in the undeterminedness of the A_L coefficients [in (BF36)], while the determinantal condition will always be fulfilled due to its construction.

ACKNOWLEDGMENTS

The authors would like to thank Dr. J. Molenaar for some valuable discussions and Dr. R. Zeller for a critical reading of this comment.

¹E. Badralex and A. J. Freeman, Phys. Rev. B **36**, 1378 (1987).

²R. G. Brown and M. Ciftan, Phys. Rev. B **27**, 4564 (1983).