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On the resolvent convergence of discrete Dirac operators on 3D cubic lattices ☆

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ABSTRACT

We prove that the discrete Dirac operators in three dimensions converge to the continuum Dirac operators in the strong resolvent sense, but not in the norm resolvent sense.

1. Introduction

Consider the free Dirac operator in three dimensions,

$$\begin{aligned} \mathbb{D}_m &= -i\alpha \cdot \nabla + m\beta \\ &= \begin{pmatrix} m & 0 & -i\partial_3 & -i\partial_1 - \partial_2 \\ 0 & m & -i\partial_1 + \partial_2 & i\partial_3 \\ -i\partial_3 & -i\partial_1 - \partial_2 & -m & 0 \\ -i\partial_1 + \partial_2 & i\partial_3 & 0 & -m \end{pmatrix}, \end{aligned} \tag{1.1}$$

where α_1, α_2, α_3 and β are Dirac matrices and $m \geq 0$ is the particle mass, and the corresponding operator discretised on a cubic lattice of mesh size $h > 0$,

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$$\mathbb{D}_{m,h} = \begin{pmatrix} m & 0 & i\partial^*_{3,h} & i\partial^*_{1,h} + \partial^*_{2,h} \\ 0 & m & i\partial^*_{1,h} - \partial^*_{2,h} & -i\partial^*_{3,h} \\ -i\partial_{3,h} & -i\partial_{1,h} - \partial_{2,h} & -m & 0 \\ -i\partial_{1,h} + \partial_{2,h} & i\partial_{3,h} & 0 & -m \end{pmatrix}. \tag{1.2}$$

In the latter operator, the partial derivatives are replaced by difference operators

$$[\partial_{j,h} f](hn) := \frac{1}{h}\Big\{f(h(n+e_j)) - f(hn)\Big\},$$
$$[\partial^*_{j,h} f](hn) := \frac{1}{h}\Big\{f(h(n-e_j)) - f(hn)\Big\}$$

where e_j is the unit vector in the direction of the jth coordinate axis. We prove that the resolvent of the embedded discrete Dirac operator $(\mathbb{D}_{m,h} \oplus \mathbf{0}_h - z)^{-1}$ strongly converges to $(\mathbb{D}_m - z)^{-1}$ in $L^2(\mathbb{R}^3)^4$ as $h \to 0$; see the beginning of Section 2 for details of the embedding. The proof presented here in the three dimensional case is simpler, shorter and more natural than in [3], where the two dimensional case was discussed. In addition, we prove that $(\mathbb{D}_{m,h} \oplus \mathbf{0}_h - z)^{-1}$ does not converge in the operator norm sense to $(\mathbb{D}_m - z)^{-1}$ as $h \to 0$. The proof of the non-convergence is an adaptation of the proof of the corresponding result in the two-dimensional case in [3]; the adaptation enables us to provide an explicit lower estimate of the norm of the resolvent difference as shown in Theorem 2.1(ii) below (compare [1, Theorems 4.11 and 5.7]). In order to get norm resolvent convergence, one has to modify the discrete Dirac operators in the cubic (resp., square) lattices. Such modifications are discussed in [1] and [2]. We remark that our imbedding operator J_h defined in the next section is different from those introduced in [1] and [2] and exactly preserves the discrete Dirac operator in $\ell^2(\mathbb{Z}^3_h)$.

We mention that using central difference operators, instead of forward and backward difference operators, to define $\mathbb{D}_{m,h}$ does not change the fundamental issue that leads to the positive lower bound for the norm of the resolvent difference in the limit (Theorem 2.1(ii)). The authors would like to thank John Pryce, Cardiff University, for suggesting the use of central difference operators.

2. Main theorem

As in [3], we make the resolvents of $\mathbb{D}_m$ and of $\mathbb{D}_{m,h}$ comparable by embedding the discrete Hilbert space $\ell^2(\mathbb{Z}^3_h)$, where $\mathbb{Z}^3_h = h\mathbb{Z}^3$, into the continuum Hilbert space $L^2(\mathbb{R}^3)$ by extending any function $f \in \ell^2(\mathbb{Z}^3_h)$ to the step function

$$(J_h f)(x) = \sum_{n\in\mathbb{Z}^3} f(hn)\, \chi_{I_{n,h}}(x) \in L^2(\mathbb{R}^3),$$

where $\chi_{I_{n,h}}$ is the characteristic function of the half-open cube

$$I_{n,h} = \{x \in \mathbb{R}^3 \mid hn_j \le x_j < h\,(n_j+1)\ (j \in \{1,2,3\})\}.$$

Clearly $\|J_h f\|^2_{L^2(\mathbb{R}^3)} = h^3 \sum_{n\in\mathbb{Z}^3} |f(hn)|^2$. The image of the embedding $L^2(\mathbb{Z}^3_h) := J_h(\ell^2(\mathbb{Z}^3_h))$ is a closed subspace of $L^2(\mathbb{R}^3)$, and $\mathbb{D}_{m,h}$ naturally acts on this subspace. Then $\mathbb{D}_{m,h} \oplus \mathbf{0}_h$ is the extension of this operator to all of $L^2(\mathbb{R}^3)$ by setting it equal to the null operator on the orthogonal complement of $L^2(\mathbb{Z}^3_h)$. The orthogonal projector P_h of $L^2(\mathbb{R}^3)$ onto $L^2(\mathbb{Z}^3_h)$ is given by (cf. [3, eq. (2.10)])

$$(P_h\varphi)(x) := \sum_{n\in\mathbb{Z}^3} \frac{1}{h^3} \int\limits_{I_{n,h}} \varphi(y)\, dy\ \chi_{I_{n,h}}(x). \tag{2.1}$$

We now state the main theorem, in which $\mathbf{B}$ denotes the Banach space of all bounded linear operators in $L^2(\mathbb{R}^3)^4$, equipped with the operator norm.

Theorem 2.1. *Let* $z \in \mathbb{C} \setminus \mathbb{R}$. *Then*
(i) $(\mathbb{D}_{m,h} \oplus \mathbf{0}_h - z)^{-1}$ *strongly converges to* $(\mathbb{D}_m - z)^{-1}$ *in* $L^2(\mathbb{R}^3)^4$ *as* $h \to 0$.

(ii) $\liminf_{h\to 0} \|(\mathbb{D}_{m,h} \oplus \mathbf{0}_h - z)^{-1} - (\mathbb{D}_m - z)^{-1}\|_{\mathbf{B}} \geq \max\left(\frac{1}{|m-z|}, \frac{1}{|m+z|}\right)$.

The proof will use the following asymptotics.

Lemma 2.1. *For* $\beta > 0$,

$$\sum_{k\in\mathbb{Z}} e^{-\beta k^2} = \sqrt{\frac{\pi}{\beta}} + O(1) \qquad (\beta \to 0), \tag{2.2}$$

$$\sum_{k=1}^{\infty} k^2\, e^{-\beta k^2} = \frac{\sqrt{\pi}}{4\sqrt{\beta}^3} + O(\beta^{-1}) \qquad (\beta \to 0). \tag{2.3}$$

Proof of Lemma 2.1. For the proof of (2.2), we split the sum into the parts with positive and with negative k (these sums are evidently equal) and the term for $k = 0$, which can be subsumed in the $O(1)$ term. For a differentiable function $f : [0, \infty) \to \mathbb{C}$, integration by parts gives the first-order Euler-Maclaurin formula

$$\sum_{k=1}^{n} f(k) = \int_0^n f(t)\, dt + \sum_{k=0}^{n-1} \int_k^{k+1} f'(t)\,(t-k)\, dt \qquad (n \in \mathbb{N}).$$

Hence

$$\sum_{k=1}^{\infty} e^{-\beta k^2} = \int_0^{\infty} e^{-\beta t^2}\, dt - \sum_{k=1}^{\infty} \int_{k-1}^{k} 2\beta t\, e^{-\beta t^2}\,(t-k)\, dt = \frac{1}{2}\sqrt{\frac{\pi}{\beta}} + O(1),$$

as $|t - k| \leq 1$ in each integral in the sum, and also

$$\begin{aligned}\sum_{k=1}^{\infty} k^2 e^{-\beta k^2} &= \int_0^{\infty} t^2\, e^{-\beta t^2}\, dt + \sum_{k=0}^{\infty} \int_k^{k+1} 2t\,(1-\beta t^2)\, e^{-\beta t^2}\,(t-k)\, dt \\ &= \frac{1}{2\beta}\int_0^{\infty} e^{-\beta t^2}\, dt + O(\beta^{-1}) = \frac{\sqrt{\pi}}{4\sqrt{\beta}^3} + O(\beta^{-1})\end{aligned}$$

by an integration by parts in the first integral and as

$$\left|\sum_{k=0}^{\infty} \int_k^{k+1} 2t\,(1-\beta t^2)\, e^{-\beta t^2}\,(t-k)\, dt\right| \leq \frac{2}{\beta}\int_0^{\infty} |s|\,|1-s^2|\, e^{-s^2}\, ds. \qquad \blacksquare$$

In the proof of Theorem 2.1, we need both the discrete Fourier transform $\mathcal{F}_h : L^2(\mathbb{Z}_h^3) \to L^2(\mathbb{T}_{1/h}^3)$ and the Fourier transform $\mathcal{F} : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$, where

$$\mathbb{T}_{1/h}^3 = [-\pi/h, \pi/h]^3 = \{\xi \in \mathbb{R}^3 \mid \max\{|\xi_1|, |\xi_2|, |\xi_3|\} \leq \pi/h\}.$$

The precise definitions of $\mathcal{F}_h$, $\mathcal{F}$ and their basic properties can be found in sections 2 and 3 of [3]. Following [3], we define the (multiplication) operators $\widehat{\mathbb{D}}_m := \mathcal{F}\,\mathbb{D}_m\overline{\mathcal{F}}$ and $\widehat{\mathbb{D}}_{m,h} := \overline{\mathcal{F}}_h D_{m,h}\mathcal{F}_h$. Since

$$\begin{aligned}[\mathcal{F}_h(\partial_{j,h} f)](\xi) &= \frac{1}{h}(e^{ih\xi_j} - 1)[\mathcal{F}_h f](\xi) \\ [\mathcal{F}_h(\partial^*_{j,h} f)](\xi) &= \frac{1}{h}(e^{-ih\xi_j} - 1)[\mathcal{F}_h f](\xi)\end{aligned} \tag{2.4}$$

we can obtain the matrix kernel $\widehat{\mathbb{D}}_{m,h}(\xi)$ in an explicit form which shows that for each $\xi \in \mathbb{R}^3$, $\big(\widehat{\mathbb{D}}_{m,h}(\xi) - \widehat{\mathbb{D}}_m(\xi)\big)\chi_{\mathbb{T}^3_{1/h}}(\xi) \to 0$ as $h \to 0$.

The orthogonal projection $Q_{1/h}$ of $L^2(\mathbb{R}^3)$ onto $L^2(\mathbb{T}^3_{1/h})$ is defined as the operator of multiplication with the characteristic function of $\mathbb{T}^3_{1/h}$. Using the projections P_h, $Q_{1/h} \in \mathbf{B}(L^2(\mathbb{R}^3))$, we extend $\mathcal{F}_h$ and its inverse $\overline{\mathcal{F}}_h$ to become elements of $\mathbf{B}(L^2(\mathbb{R}^3))$ by setting

$$\mathcal{F}_h := Q_{1/h}\,\mathcal{F}_h P_h, \quad \overline{\mathcal{F}}_h := P_h \overline{\mathcal{F}}_h Q_{1/h}. \tag{2.5}$$

It is clear that

$$\overline{\mathcal{F}}_h \mathcal{F}_h = P_h, \qquad \mathcal{F}_h \overline{\mathcal{F}}_h = Q_{1/h}, \tag{2.6}$$

and

$$P_h^\perp \overline{\mathcal{F}}_h = \mathbf{0}, \quad Q_{1/h}^\perp \mathcal{F}_h = \mathbf{0}. \tag{2.7}$$

Proof of Theorem 2.1. (i) Since $\mathcal{S}(\mathbb{R}^3)^4$, the Schwartz space of rapidly decreasing functions, is dense in $L^2(\mathbb{R}^3)^4$ and

$$\|(\mathbb{D}_{m,h} - z)^{-1} \oplus \mathbf{0}_h\|_{\mathbf{B}} \le 1/|\mathfrak{Im}\, z|, \tag{2.8}$$

it is sufficient to prove that

$$\lim_{h\to 0} \|\big\{(\mathbb{D}_{m,h} - z)^{-1} \oplus \mathbf{0}_h - (\mathbb{D}_m - z)^{-1}\big\}\varphi\|_{[L^2]^4} = 0$$

for $\varphi \in \mathcal{S}(\mathbb{R}^3)^4$. We begin with

$$\begin{aligned}&\big\{(\mathbb{D}_{m,h} - z)^{-1} \oplus \mathbf{0}_h - (\mathbb{D}_m - z)^{-1}\big\}\varphi - \overline{\mathcal{F}}(\widehat{\mathbb{D}}_m - z)^{-1}\mathcal{F}\varphi \\ &\quad = \overline{\mathcal{F}}_h\big\{(\widehat{\mathbb{D}}_{m,h} - z)^{-1} \oplus \mathbf{0}_h\big\}(\mathcal{F}_h - \mathcal{F})\varphi \\ &\qquad + (\overline{\mathcal{F}}_h - \overline{\mathcal{F}})\big\{(\widehat{\mathbb{D}}_{m,h} - z)^{-1} \oplus \mathbf{0}_h\big\}\mathcal{F}\varphi \\ &\qquad + \overline{\mathcal{F}}\big\{(\widehat{\mathbb{D}}_{m,h} - z)^{-1} \oplus \mathbf{0}_h - (\widehat{\mathbb{D}}_m - z)^{-1}\big\}\mathcal{F}\varphi.\end{aligned} \tag{2.9}$$

The L^2 norm of the first term on the right hand side of (2.9) can be estimated by

$$\|(\widehat{\mathbb{D}}_{m,h} - z)^{-1} \oplus \mathbf{0}_h\|_{\mathbf{B}} \|(\mathcal{F}_h - \mathcal{F})\varphi\|_{L^2(\mathbb{R}^3)^4} \le \Big(\frac{1}{|\mathfrak{Im}\, z|}\Big)\|(\mathcal{F}_h - \mathcal{F})\varphi\|_{L^2(\mathbb{R}^3)^4}$$

which, by [3, Lemma 3.6], tends to 0 as $h \to 0$. The second term on the right hand side of (2.9) can be written as

$$\begin{aligned}&(\overline{\mathcal{F}}_h - \overline{\mathcal{F}})\big\{(\widehat{\mathbb{D}}_{m,h} - z)^{-1} \oplus \mathbf{0}_h\big\}\mathcal{F}\varphi \\ &\quad = (\overline{\mathcal{F}}_h - \overline{\mathcal{F}})\big\{(\widehat{\mathbb{D}}_m - z)^{-1} \oplus \mathbf{0}_h\big\}\mathcal{F}\varphi \\ &\qquad + (\overline{\mathcal{F}}_h - \overline{\mathcal{F}})\big\{(\widehat{\mathbb{D}}_{m,h} - z)^{-1} \oplus \mathbf{0}_h - (\widehat{\mathbb{D}}_m - z)^{-1}\big\}\mathcal{F}\varphi,\end{aligned} \tag{2.10}$$

where, by [3, Lemma 3.5], the L^2 norm of the term (2.10) tends to 0 as $h \to 0$. Combining all the arguments above, we infer that

$$\begin{aligned}&\limsup_{h\to 0} \|\{(\mathbb{D}_{m,h} - z)^{-1} \oplus \mathbf{0}_h - (\mathbb{D}_m - z)^{-1}\}\varphi\|_{L^2(\mathbb{R}^3)^4} \\ &\quad \le 2 \limsup_{h\to 0} \|\{(\widehat{\mathbb{D}}_{m,h} - z)^{-1} \oplus \mathbf{0}_h - (\widehat{\mathbb{D}}_m - z)^{-1}\}\mathcal{F}\varphi\|_{L^2(\mathbb{R}^3)^4}.\end{aligned}$$

We finish the proof of statement (i) by showing that

$$\lim_{h\to 0} \|\{(\widehat{\mathbb{D}}_{m,h} - z)^{-1} \oplus \mathbf{0}_h - (\widehat{\mathbb{D}}_m - z)^{-1}\}\mathcal{F}\varphi\|_{L^2(\mathbb{R}^3)^4} = 0. \tag{2.11}$$

The expression in (2.11) is estimated by

$$\begin{aligned}&\lim_{h\to 0} \|\{(\widehat{\mathbb{D}}_{m,h} - z)^{-1} \oplus \mathbf{0}_h - (\widehat{\mathbb{D}}_m - z)^{-1}\}Q_{1/h}\mathcal{F}\varphi\|_{L^2(\mathbb{R}^3)^4} \\ &\quad + \lim_{h\to 0} \|\{(\widehat{\mathbb{D}}_m - z)^{-1}\}Q_{1/h}^{\perp}\mathcal{F}\varphi\|_{L^2(\mathbb{R}^3)^4}.\end{aligned} \tag{2.12}$$

The second term of (2.12) equals 0 since

$$(\widehat{\mathbb{D}}_m(\xi) - z)^{-1} = (|\xi|^2 + m^2 - z^2)^{-1}(\widehat{\mathbb{D}}_m(\xi) + z).$$

The first term of (2.12) is bounded by

$$\begin{aligned}&\lim_{h\to 0} \|(\widehat{\mathbb{D}}_{m,h} - z)^{-1}(\widehat{\mathbb{D}}_m - \widehat{\mathbb{D}}_{m,h})(\widehat{\mathbb{D}}_m - z)^{-1}Q_{1/h}\mathcal{F}\varphi\|_{L^2(\mathbb{R}^3)^4} \\ &\quad \le \frac{1}{|\mathfrak{Im}\, z|} \lim_{h\to 0} \left\{ \int_{\mathbb{R}^3} \left| (\widehat{\mathbb{D}}_m(\xi) - \widehat{\mathbb{D}}_{m,h}(\xi))\chi_{\mathbb{T}^3_{1/h}}(\xi)(\widehat{\mathbb{D}}_m(\xi) - z)^{-1}[\mathcal{F}\varphi](\xi)\right|^2_{\mathbb{C}^4} d\xi \right\}^{1/2}.\end{aligned}$$

Note that $\mathcal{F}\varphi$ on the right hand side of the above inequality belongs to $\mathcal{S}(\mathbb{R}^3)^4$. In a similar manner to [3, Lemma 4.2], one can show that

$$\left\|(\widehat{\mathbb{D}}_{m,h}(\xi) - \widehat{\mathbb{D}}_m(\xi))\chi_{\mathbb{T}^3_{1/h}}(\xi)\right\|_{\mathbf{B}(\mathbb{C}^4)} \le \frac{h}{2}|\xi|^2.$$

Equation (2.11) then follows by the Lebesgue dominated convergence theorem.

(ii) Let $u_h = (y_h, 0, 0, 0)^T \in L^2(\mathbb{R}^3)^4$,

$$y_h(x) = h^{\frac{3}{4}}\, e^{i\frac{\pi}{2h}(x_1 - x_2)}\, e^{-h(x_1^2+x_2^2+x_3^2)} \quad (x \in \mathbb{R}^3),$$

for all $h > 0$; then $\|u_h\|_{L^2(\mathbb{R}^3)^4} = \left(\frac{\pi}{2}\right)^{\frac{3}{4}}$.

As the function $e^{-x^2/2}$ ($x \in \mathbb{R}$) is its own Fourier transform, we find for all $\xi \in \mathbb{R}^3$

$$(\mathcal{F}\, y_h)(\xi) = \frac{1}{(4h)^{\frac{3}{4}}}\, e^{-\frac{1}{4h}[(\xi_1 - \frac{\pi}{2h})^2 + (\xi_2 + \frac{\pi}{2h})^2 + \xi_3^2]}.$$

Let $z \in \mathbb{C} \setminus \mathbb{R}$. In the following, we show that $(\mathbb{D}_m - z)\, u_h$ tends to 0 as $h \to 0$ (step 1), whereas the norm of $(\mathbb{D}_{m,h} \oplus \mathbf{0}_h - z)^{-1}\, u_h$ remains bounded from below by $|m - z|^{-1}$, up to an error that vanishes in the limit (step 3). In step 2, we prepare application of the embedded discrete Dirac operator by calculating the projection $P_h y_h$, up to small error.

Step 1. Applying the Fourier transformation to the Dirac operator (1.1) and taking the matrix inverse, we find

$$(\mathbb{D}_m - z)^{-1} u_h = \overline{\mathcal{F}} \frac{1}{m^2 - z^2 + \xi_1^2 + \xi_2^2 + \xi_3^2} \times \begin{pmatrix} m+z & 0 & \xi_3 & \xi_1 - i\xi_2 \\ 0 & m+z & \xi_1 + i\xi_2 & -\xi_3 \\ \xi_3 & \xi_1 - i\xi_2 & -m+z & 0 \\ \xi_1 + i\xi_2 & -\xi_3 & 0 & -m+z \end{pmatrix} \begin{pmatrix} \mathcal{F} y_h \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

As the Fourier transform is an isometry on $L^2(\mathbb{R}^3)$,

$$\|(\mathbb{D}_m - z)^{-1} u_h\|^2_{L^2(\mathbb{R}^3)^4} = \int_{\mathbb{R}^3} \frac{|m+z|^2 + \xi_1^2 + \xi_2^2 + \xi_3^2}{|m^2 - z^2 + \xi_1^2 + \xi_2^2 + \xi_3^2|^2} \times \frac{1}{(4h)^{\frac{3}{2}}} e^{-[(\xi_1 - \frac{\pi}{2h})^2 + (\xi_2 + \frac{\pi}{2h})^2 + \xi_3^2]/2h} \, d\xi.$$

Now we observe that there is a constant $C_z > 0$ (which may depend on z) such that

$$\frac{|m+z|^2 + \xi_1^2 + \xi_2^2 + \xi_3^2}{|m^2 - z^2 + \xi_1^2 + \xi_2^2 + \xi_3^2|} \le C_z \qquad (\xi \in \mathbb{R}^3),$$

since the denominator is bounded below by a positive constant and the fraction tends to 1 as $|\xi| \to \infty$. Hence

$$\begin{aligned} \|(\mathbb{D}_m - z)^{-1} u_h\|^2_{L^2(\mathbb{R}^3)^4} &\le C_z \int_{\mathbb{R}^3} \frac{e^{-[(\xi_1 - \frac{\pi}{2h})^2 + (\xi_2 + \frac{\pi}{2h})^2 + \xi_3^2]/2h}}{(4h)^{\frac{3}{2}} |m^2 - z^2 + \xi_1^2 + \xi_2^2 + \xi_3^2|} \, d\xi \\ &= \frac{C_z}{8} \int_{\mathbb{R}^3} \frac{e^{-(\zeta_1^2 + \zeta_2^2 + \zeta_3^2)/2}}{|m^2 - z^2 + (\sqrt{h}\zeta_1 + \frac{\pi}{2h})^2 + (\sqrt{h}\zeta_2 - \frac{\pi}{2h})^2 + h\zeta_3^2|} \, d\zeta. \end{aligned}$$

The last integral converges to 0 as $h \to 0$ by dominated convergence, as the integrand tends to 0 pointwise and can be bounded above by an h-independent multiple of $e^{-(\zeta_1^2+\zeta_2^2+\zeta_3^2)/2}$. We have thus established that

$$\lim_{h \to 0} \|(\mathbb{D}_m - z)^{-1} u_h\|_{L^2(\mathbb{R}^3)^4} = 0.$$

Step 2. Before we can apply the discrete Dirac operator (1.2), we need to project u_h into the subspace $L^2(\mathbb{Z}_h^3)^4$. By equation (2.1), the projection is given by $P_h y_h = \sum_{n \in \mathbb{Z}^3} \widetilde{y}_h(hn) \chi_{I_{n,h}}$, where

$$\widetilde{y}_h(hn) = h^{\frac{3}{4}} \left(\int_{n_1}^{n_1+1} e^{i\frac{\pi}{2}t} \, e^{-h^3 t^2} \, dt \right) \left(\int_{n_2}^{n_2+1} e^{-i\frac{\pi}{2}t} \, e^{-h^3 t^2} \, dt \right) \left(\int_{n_3}^{n_3+1} e^{-h^3 t^2} \, dt \right)$$

for all $n \in \mathbb{Z}^3$. By an integration by parts, we find for all $k \in \mathbb{Z}$

$$\int_k^{k+1} e^{\pm i\frac{\pi}{2}t} e^{-h^3 t^2} \, dt = \frac{2}{\pi}(1 \pm i) \, e^{\pm i\frac{\pi}{2}k} e^{-h^3 k^2} + \frac{4h^3}{\pi} K^{\pm}_{k,h} \tag{2.13}$$

with

$$K_{k,h}^{\pm} = \frac{e^{\pm i\frac{\pi}{2}k}}{2h^3}\,(e^{-h^3(k+1)^2} - e^{-h^3k^2}) \mp i\int_k^{k+1} e^{\pm i\frac{\pi}{2}t}\,t\,e^{-h^3t^2}\,dt$$
$$= \int_k^{k+1} e^{\pm i\frac{\pi}{2}k}\,t\,e^{-h^3t^2}dt \mp i\int_k^{k+1} e^{\pm i\frac{\pi}{2}t}\,t\,e^{-h^3t^2}\,dt.$$

Noting that $xe^{-x^2/2} \le \frac{1}{\sqrt{e}}$ $(x \ge 0)$, we obtain the estimate

$$\sum_{k\in\mathbb{Z}} |h^{\frac{3}{2}} K_{k,h}^{\pm}|^2 \le \sum_{k\in\mathbb{Z}} \left(2\int_k^{k+1} h^{\frac{3}{2}}\,|t|\,e^{-(h^{\frac{3}{2}}|t|)^2/2}\,e^{-h^3t^2/2}\,dt\right)^2 \tag{2.14}$$
$$\le \frac{4}{e}\sum_{k\in\mathbb{Z}}\left(\int_k^{k+1} e^{-h^3t^2/2}\,dt\right)^2$$
$$\le \frac{8}{e}\sum_{k=0}^{\infty} e^{-h^3k^2} = \frac{4\sqrt{\pi}}{eh^{\frac{3}{2}}} + O(1) \qquad (h \to 0)$$

by (2.2). Similarly,

$$\int_k^{k+1} e^{-h^3t^2}\,dt = e^{-h^3k^2} + 2h^3 K_{k,h}^0 \tag{2.15}$$

with

$$K_{k,h}^0 = \frac{1}{2h^3}\int_k^{k+1} (e^{-h^3t^2} - e^{-h^3k^2})\,dt = -\int_k^{k+1}\int_k^{t} s\,e^{-h^3s^2}\,ds\,dt$$
$$= -\int_k^{k+1} (k+1-s)\,s\,e^{-h^3s^2}\,ds,$$

and we have the estimate

$$\sum_{k\in\mathbb{Z}} |h^{\frac{3}{2}} K_{k,h}^0|^2 \le \sum_{k\in\mathbb{Z}} \left(\int_k^{k+1} h^{\frac{3}{2}}\,|s|\,e^{-(h^{\frac{3}{2}}|s|)^2/2}\,e^{-h^3s^2/2}\,ds\right)^2 \tag{2.16}$$
$$\le \frac{1}{e}\sum_{k\in\mathbb{Z}}\left(\int_k^{k+1} e^{-h^3s^2/2}\,ds\right)^2 \le \frac{\sqrt{\pi}}{eh^{\frac{3}{2}}} + O(1)$$

$(h \to 0)$. Using equations (2.13) and (2.15), we can write $\widetilde{y}_h(hn)$ in the form

$$\widetilde{y}_h(hn) = h^{\frac{3}{4}}\left(\frac{2}{\pi}\,(1+i)\,e^{i\frac{\pi}{2}n_1}e^{-h^3n_1^2} + \frac{4h^3}{\pi}\,K_{n_1,h}^{+}\right)$$
$$\times\left(\frac{2}{\pi}\,(1-i)\,e^{-i\frac{\pi}{2}n_2}e^{-h^3n_2^2} + \frac{4h^3}{\pi}\,K_{n_2,h}^{-}\right)\left(e^{h^3n_3^2} + 2h^3K_{n_3,h}^0\right)$$

$$= \frac{8}{\pi^2} y_h(nh) + \sum_{j=1}^{7} R_{j,n,h}$$

where

$$R_{1,n,h} = h^{3+\frac{3}{4}} \frac{16}{\pi^2} e^{i\frac{\pi}{2}(n_1-n_2)} e^{-h^3(n_1^2+n_2^2)} K^0_{n_3,h},$$
$$R_{2,n,h} = h^{3+\frac{3}{4}} \frac{8}{\pi^2} (1+i) e^{i\frac{\pi}{2}n_1} e^{-h^3(n_1^2+n_3^2)} K^-_{n_2,h},$$
$$R_{3,n,h} = h^{3+\frac{3}{4}} \frac{8}{\pi^2} (1-i) e^{-i\frac{\pi}{2}n_2} e^{-h^3(n_2^2+n_3^2)} K^+_{n_1,h},$$
$$R_{4,n,h} = h^{6+\frac{3}{4}} \frac{16}{\pi^2} (1+i) e^{i\frac{\pi}{2}n_1} e^{-h^3 n_1^2} K^-_{n_2,h} K^0_{n_3,h},$$
$$R_{5,n,h} = h^{6+\frac{3}{4}} \frac{16}{\pi^2} (1-i) e^{-i\frac{\pi}{2}n_2} e^{-h^3 n_2^2} K^+_{n_1,h} K^0_{n_3,h},$$
$$R_{6,n,h} = h^{6+\frac{3}{4}} \frac{16}{\pi^2} e^{-h^3 n_3^2} K^+_{n_1,h} K^-_{n_2,h},$$
$$R_{7,n,h} = h^{9+\frac{3}{4}} \frac{32}{\pi^2} K^+_{n_1,h} K^-_{n_2,h} K^0_{n_3,h}.$$

With the notation

$$R_h^{(j)} := \sum_{n\in\mathbb{Z}^3} R_{j,n,h}\, \chi_{I_{n,h}} \qquad (j \in \{1, \cdots, 7\}),$$

we embed the remainder term into $L^2(\mathbb{Z}_h^3)$ by defining $R_h = \sum_{j=1}^7 R_h^{(j)}$ and also set $(y_h)_h = J_h y_h$; then

$$P_h\, y_h = \frac{8}{\pi^2} (y_h)_h + R_h. \tag{2.17}$$

Each $R_h^{(j)}$, where $j \in \{1, \ldots, 7\}$, can be estimated as follows.

$$\begin{aligned} \|R_h^{(1)}\|^2_{L^2(\mathbb{Z}_h^3)} &= h^{3+\frac{9}{2}} \frac{256}{\pi^4} \left(\sum_{n_1\in\mathbb{Z}} e^{-2h^3 n_1^2}\right) \left(\sum_{n_2\in\mathbb{Z}} e^{-2h^3 n_2^2}\right) \left(\sum_{n_3\in\mathbb{Z}} |h^{\frac{3}{2}} K^0_{n_3,h}|^2\right) \\ &\le h^{3+\frac{9}{2}} \frac{256}{\pi^4} \left(\sqrt{\frac{\pi}{2h^3}} + O(1)\right)^2 \left(\frac{\sqrt{\pi}}{e h^{\frac{3}{2}}} + O(1)\right) \\ &= \frac{128}{\sqrt{\pi}\, e} h^3 + O(h^{\frac{9}{2}}), \end{aligned}$$

where we used the first asymptotic formula in Lemma 2.1 and the estimate (2.16). Analogously,

$$\begin{aligned} \|R_h^{(2)}\|^2_{L^2(\mathbb{Z}_h^3)} &\le h^{3+3+\frac{3}{2}} \frac{128}{\pi^4} \left(\sqrt{\frac{\pi}{2h^3}} + O(1)\right)^2 \left(\frac{4\sqrt{\pi}}{e\, h^{\frac{3}{2}}} + O(1)\right) \\ &= \frac{256}{\pi^{\frac{5}{2}} e} h^3 + O(h^{\frac{9}{2}}) \end{aligned}$$

using the estimate (2.14); the same estimate holds for $\|R_h^{(3)}\|^2_{L^2(\mathbb{Z}_h^3)}$. Further,

$$\begin{aligned}\|R_h^{(4)}\|^2_{L^2(\mathbb{Z}_h^3)} &\le h^{3+6+\frac{3}{2}}\,\frac{512}{\pi^4}\left(\sqrt{\frac{\pi}{2h^3}}+O(1)\right)\left(\frac{4\sqrt{\pi}}{e\,h^{\frac{3}{2}}}+O(1)\right)\left(\frac{\sqrt{\pi}}{e\,h^{\frac{3}{2}}}+O(1)\right)\\ &= \frac{1024}{\sqrt{2}\,\pi^{\frac{5}{2}}e^2}\,h^6+O(h^{\frac{15}{2}}),\end{aligned}$$

and the same estimate holds for $\|R_h^{(5)}\|^2_{L^2(\mathbb{Z}_h^3)}$. We find

$$\begin{aligned}\|R_h^{(6)}\|^2_{L^2(\mathbb{Z}_h^3)} &\le h^{3+6+\frac{3}{2}}\,\frac{256}{\pi^4}\left(\sqrt{\frac{\pi}{2h^3}}+O(1)\right)\left(\frac{4\sqrt{\pi}}{e\,h^{\frac{3}{2}}}+O(1)\right)^2\\ &= \frac{4096}{\sqrt{2}\,\pi^{\frac{5}{2}}e^2}\,h^6+O(h^{\frac{15}{2}})\end{aligned}$$

and finally

$$\begin{aligned}\|R_h^{(7)}\|^2_{L^2(\mathbb{Z}_h^3)} &\le h^{3+9+\frac{3}{2}}\,\frac{1024}{\pi^4}\left(\frac{4\sqrt{\pi}}{e\,h^{\frac{3}{2}}}+O(1)\right)^2\left(\frac{\sqrt{\pi}}{e\,h^{\frac{3}{2}}}+O(1)\right)\\ &= \frac{16384}{\pi^{\frac{5}{2}}e^3}\,h^9+O(h^{\frac{21}{2}}).\end{aligned}$$

In total, this gives $\|R_h\|_{L^2(\mathbb{Z}_h^3)} = O(h^{\frac{3}{2}})$ as $h \to 0$. By (2.2), the first term in (2.17) satisfies

$$\|\frac{8}{\pi^2}(y_h)_h\|^2_{L^2(\mathbb{Z}_h^3)} = h^{3+\frac{3}{2}}\,\frac{64}{\pi^4}\left(\sqrt{\frac{\pi}{2h^3}}+O(1)\right)^3,$$

so $\|\frac{8}{\pi^2}(y_h)_h\|_{L^2(\mathbb{Z}_h^3)} = \frac{8}{\pi^{\frac{5}{4}}2^{\frac{3}{4}}} + O(h^{\frac{3}{2}})$.

Step 3. We now apply the discrete Dirac operator,

$$(\mathbb{D}_{m,h}-z)\begin{pmatrix}(y_h)_h\\0\\0\\0\end{pmatrix} = \begin{pmatrix}(m-z)\,(y_h)_h\\0\\-i\partial_{3,h}(y_h)_h\\(-i\partial_{1,h}+\partial_{2,h})(y_h)_h\end{pmatrix}. \tag{2.18}$$

Here

$$\begin{aligned}D_{1,h}(nh) &:= -i\partial_{3,h}(y_h)_h(nh) \qquad (n\in\mathbb{Z}^3)\\ &= -ih^{-\frac{1}{4}}e^{i\frac{\pi}{2}(n_1-n_2)}e^{-h^3(n_1^2+n_2^2+n_3^2)}\left(e^{-h^3(2n_3+1)}-1\right);\end{aligned}$$

noting that

$$\left|e^{-h^3(2k+1)}-1\right| = \left|-h^3\int_0^{2k+1}e^{-h^3t}\,dt\right| \le (2k+1)\,h^3$$

and $(2k+1)^2 \le 1+8k^2$ for $k\in\mathbb{N}_0$, we find, using both asymptotic formulae in Lemma 2.1,

$$\begin{aligned}\|D_{1,h}\|^2_{L^2(\mathbb{Z}_h^3)} &\le h^{3-\frac{1}{2}}\left(\sum_{n_1\in\mathbb{Z}}e^{-2h^3n_1^2}\right)\left(\sum_{n_2\in\mathbb{Z}}e^{-2h^3n_2^2}\right)2\left(\sum_{n_3\in\mathbb{N}_0}e^{-2h^3n_3^2}(2n_3+1)^2h^6\right)\\ &\le h^{3-\frac{1}{2}+6}\left(\frac{\pi}{2h^3}+O(\frac{1}{h^{\frac{3}{2}}})\right)\left(\frac{\sqrt{2\pi}}{h^{\frac{9}{2}}}+O(\frac{1}{h^3})\right)\end{aligned}$$

$$= \frac{\sqrt{\pi}^3}{\sqrt{2}}\, h + O(h^{\frac{5}{2}}) \qquad (h \to 0).$$

Hence $\|D_{1,h}\|_{L^2(\mathbb{Z}_h^3)} \leq \left(\frac{\pi^3}{2}\right)^{\frac{1}{4}} \sqrt{h} + O(h^2)$. Similarly, we find for

$$\begin{aligned} D_{2,h}(hn) &:= (-i\partial_{1,h} + \partial_{2,h})(y_h)_h(hn) \\ &= (-i\partial_{1,h} + \partial_{2,h}) h^{\frac{3}{4}}\, e^{i\frac{\pi}{2}(n_1-n_2)} e^{-h^3(n_1^2+n_2^2+n_3^2)} \\ &= h^{-\frac{1}{4}} e^{i\frac{\pi}{2}(n_1-n_2)} e^{-h^3(n_1^2+n_2^2+n_3^2)} \left((e^{-h^3(2n_1+1)} - 1) - i\,(e^{-h^3(2n_2+1)} - 1) \right) \end{aligned}$$

the norm estimate $\|D_{2,h}\|_{L^2(\mathbb{Z}_h^3)} \leq (2\pi)^{\frac{3}{4}} \sqrt{h} + O(h^2)$.

To complete the proof, we first note that

$$(\mathbb{D}_{m,h} \oplus \mathbf{0}_h - z)^{-1} = (\mathbb{D}_{m,h} - z)^{-1} \oplus \left(-\frac{1}{z}\right).$$

By equations (2.17) and (2.18),

$$(\mathbb{D}_{m,h} - z) P_h u_h = \frac{8}{\pi^2}(m-z)\,(u_h)_h + \frac{8}{\pi^2} \begin{pmatrix} 0 \\ 0 \\ D_{1,h} \\ D_{2,h} \end{pmatrix} + (\mathbb{D}_{m,h} - z) \begin{pmatrix} R_h \\ 0 \\ 0 \\ 0 \end{pmatrix},$$

and, using (2.17) again in the first term on the right hand side and applying $\frac{1}{m-z}(\mathbb{D}_{m,h} - z)^{-1}$ on both sides of the equation, we find

$$\begin{aligned} (\mathbb{D}_{m,h} - z)^{-1} P_h u_h = \frac{1}{m-z}\, P_h u_h - \frac{8}{\pi^2}\, \frac{1}{m-z}\, (\mathbb{D}_{m,h} - z)^{-1} \begin{pmatrix} 0 \\ 0 \\ D_{1,h} \\ D_{2,h} \end{pmatrix} \\ - \frac{1}{m-z} \begin{pmatrix} R_h \\ 0 \\ 0 \\ 0 \end{pmatrix} + (\mathbb{D}_{m,h} - z)^{-1} \begin{pmatrix} R_h \\ 0 \\ 0 \\ 0 \end{pmatrix}. \end{aligned}$$

Using the estimate (2.8), we hence obtain

$$\begin{aligned} &\left\| (\mathbb{D}_{m,h} - z)^{-1} P_h u_h - \frac{1}{m-z}\, P_h u_h \right\|_{L^2(\mathbb{R}^3)^4} \\ &\leq \frac{8\sqrt{\|D_{1,h}\|^2_{L^2(\mathbb{Z}_h^3)} + \|D_{2,h}\|^2_{L^2(\mathbb{Z}_h^3)}}}{|m-z|\,|\mathfrak{Im}\, z|\,\pi^2} + \left(\frac{1}{|m-z|} + \frac{1}{|\mathfrak{Im}\, z|}\right) \|R_h\|_{L^2(\mathbb{Z}_h^3)} \to 0 \end{aligned}$$

as $h \to 0$ by our remainder term estimates. Thus

$$\begin{aligned} &\|u_h\|_{L^2(\mathbb{R}^3)^4} \|(\mathbb{D}_{m,h} \oplus \mathbf{0}_h - z)^{-1} - (\mathbb{D}_m - z)^{-1}\|_{\mathbf{B}} \\ &\geq \|(\mathbb{D}_{m,h} - z)^{-1} P_h u_h - \frac{1}{z}\,(1 - P_h) u_h\|_{L^2(\mathbb{R}^3)^4} - \|(\mathbb{D}_m - z)^{-1} u_h\|_{L^2(\mathbb{R}^3)^4} \\ &= \left\{ \|(\mathbb{D}_{m_h} - z)^{-1} P_h u_h\|^2_{L^2(\mathbb{R}^3)^4} + \frac{1}{|z|^2}\, \|(1 - P_h) u_h\|^2_{L^2(\mathbb{R}^3)^4} \right\}^{1/2} + o(1) \\ &\geq \|(\mathbb{D}_{m,h} - z)^{-1}\, P_h\, u_h\|_{L^2(\mathbb{R}^3)^4} + o(1) \end{aligned}$$

$$= \left\| \frac{1}{m-z} P_h u_h \right\|_{L^2(\mathbb{R}^3)^4} + o(1) = \frac{1}{|m-z|} \|u_h\|_{L^2(\mathbb{R}^3)^4} + o(1) \qquad (h \to 0),$$

where we used in the last step the strong convergence of P_h to the identity operator., see [3, Lemma 3.3]. As $\|u_h\|_{L^2(\mathbb{R}^3)^4}$ is independent of h, it follows that

$$\liminf_{h\to 0} \|(\mathbb{D}_{m,h} \oplus \mathbf{0}_h - z)^{-1} - (\mathbb{D}_m - z)^{-1}\|_{\mathbf{B}} \geq \frac{1}{|m-z|}.$$

The second lower bound in statement (ii) follows analogously starting from $u_h = (0, 0, y_h, 0)^T$. ■

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