A note on the nonrelativistic limit of Dirac operators and spectral concentration

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(Communicated by Heisuke HIRONAKA, M. J. A., Dec. 12, 2005)

Abstract: We study the nonrelativistic limit of Dirac operators from the viewpoint of the spectral relationship between Dirac operators and Pauli operators. We show that Dirac operators have spectral concentration about eigenvalues of Pauli operators for a large class of magnetic fields and electric potentials diverging at infinity.

Key words: Dirac operators; nonrelativistic limit; Pauli operators; spectral concentration.

1. Introduction. We consider the Dirac operator

$$H_c := c\sum_{j=1}^{3}\alpha_j D_j + mc^2\beta + V(x),$$

$$D_j = -i\frac{\partial}{\partial x_j} - b_j(x),$$

in the Hilbert space $\mathcal{H} := \mathbf{h}^4$ with $\mathbf{h} = L^2(\mathbf{R}^3)$, where $c > 0$ is the velocity of light, $m > 0$ the rest mass of the particle and

$$\alpha_j := \begin{pmatrix} \mathbf{0} & \sigma_j \\ \sigma_j & \mathbf{0} \end{pmatrix}, \quad \beta := \begin{pmatrix} I_2 & \mathbf{0} \\ \mathbf{0} & -I_2 \end{pmatrix}$$

with the 2×2 identity matrix I_2 and Pauli matrices

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

$$\sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Here we keep the anti-commutation relation

$$(1) \qquad \alpha_j\alpha_k + \alpha_k\alpha_j = 2\delta_{jk}I_4, \quad \beta\alpha_j = -\alpha_j\beta$$

in mind. Each $b_j(x)$ is assumed to be a real-valued smooth function, and $V(x)$ is a 4×4 Hermitian matrix-valued function. Throughout this note we assume that each component of $V(x)$ is continuous in $\mathbf{R}^3$, although some singularities may be allowed. Then H_c on $C_0^\infty(\mathbf{R}^3)^4$ is essentially self-adjoint in $\mathcal{H}$. We denote its unique self-adjoint extension by H_c again. In this paper we assume that V has the form

$$V(x) := \begin{pmatrix} V_+(x) & \mathbf{0} \\ \mathbf{0} & V_-(x) \end{pmatrix},$$

with 2×2 Hermitian matrix-valued functions $V_\pm(x)$ and consider the corresponding Pauli operators

$$S_\pm := \pm\frac{1}{2m}(\sigma \cdot D)^2 + V_\pm(x)$$

$$= \pm\frac{1}{2m}\sum_{j=1}^{3} D_j^2 \mp \frac{1}{2m}(B(x)\cdot\sigma) + V_\pm(x)$$

acting on $\mathbf{h}^2 = L^2(\mathbf{R}^3)^2$, where

$$\sigma \cdot D := \sum_{j=1}^{3}\sigma_j D_j, \quad B(x)\cdot\sigma := \sum_{j=1}^{3} B_j(x)\sigma_j,$$

$$(B_1(x), B_2(x), B_3(x)) = \mathrm{curl}(b_1(x), b_2(x), b_3(x)).$$

The nonrelativistic limit of Dirac operators has been intensively studied by many authors from various points of view and it has been shown that the dynamics e^{-itH_c}, the resolvent $(H_c - z)^{-1}$ and the scattering operator for H_c converge as $c \to \infty$ to the corresponding objects for the corresponding Schrödinger operators (see, e.g., Cirincione-Chernoff [3], Hunziker [6], Yajima [17], respectively). In this paper we study the relation between the spectra of H_c and

$$S := \begin{pmatrix} S_+ & \mathbf{0} \\ \mathbf{0} & S_- \end{pmatrix},$$

another important object.

We consider a simple case of scalar potentials $V(x) = v(x)I_4$, that is, $V_\pm(x) = v(x)I_2$ and $b_j(x) \equiv 0$ $(1 \le j \le 3)$. If $v(x) \in C^0(\mathbf{R}^3)$ satisfies

2000 Mathematics Subject Classification. Primary 35Q40; Secondary 35P99, 81Q10.

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(2) $$v(x) \to +\infty \quad (|x| \to \infty),$$

it is well known that $S_+ = -(1/2m)\Delta + v(x)$ on $C_0^\infty(\mathbf{R}^3)^2$ is essentially self-adjoint. The spectrum of S_+ is purely discrete, that is, the spectrum $\sigma(S_+)$ consists of eigenvalues

$$\lambda_1 < \lambda_2 < \cdots \lambda_n < \cdots \to +\infty \quad (n \to \infty)$$

with finite multiplicity (Reed-Simon [11, Theorem XIII.67]). On the other hand, $\sigma(H_c)$ is purely (absolutely) continuous and covers the whole real line (cf. Kalf-Ōkaji-Yamada [9], Schmidt-Yamada [12]).

There are several works which explain how these spectra of different natures of H_c and S_+ are related. Titchmarsh [14], Grigore-Nenciu-Purice [4] and Amour-Brummelhuis-Nourrigat [2] explain this by proving that resonances of H_c converge as $c \to \infty$ to isolated eigenvalues of corresponding Schrödinger operators and Veselić [16] does this in terms of spectral concentration. In this paper we generalize Veselić's [16] result to the case that electric fields V are in more general class and that magnetic fields are present.

2. The nonrelativistic limit. In this section we give a theorem concerning the nonrelativistic limit of H_c. We introduce some notations. Let $E_c(\lambda)$ and $E_\pm(\lambda)$ be the right-continuous spectral families of self-adjoint operators H_c and $SQ_\pm$, respectively, where $Q_\pm := (I \pm \beta)/2$, that is,

$$H_c = \int_{-\infty}^{+\infty} \lambda\, dE_c(\lambda), \quad SQ_\pm = \int_{-\infty}^{+\infty} \lambda\, dE_\pm(\lambda),$$
$$SQ_+ = \begin{pmatrix} S_+ & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad SQ_- = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & S_- \end{pmatrix}.$$

Theorem 2.1. *Assume that $V_\pm(x) \in C^0$ and $b_j(x) \in C^3$ on $\mathbf{R}^3$. Suppose*

(i) *S_+ (or S_-) on $C_0^\infty(\mathbf{R}^3)^2$ is essentially self-adjoint in $\mathbf{h}^2$,*

(ii) *λ is an isolated eigenvalue of S_+ (or S_-) with finite multiplicity in some interval $I = (a, b)$ such that*

$$(a,b) \cap \sigma(S_+) = \{\lambda\} \quad (\textit{or } (a,b) \cap \sigma(S_-) = \{\lambda\}),$$

where $\sigma(S_\pm)$ is the spectrum of $S_\pm$. Moreover, neither a nor b is an eigenvalue of S_+ (or S_-),

(iii) *every eigenfunction u of S_+ (or S_-) corresponding to λ satisfies $(\sigma \cdot D)u \in \mathbf{h}^2$ and*

$$V_-(\sigma \cdot D)u \in \mathbf{h}^2 \quad (\textit{or } V_+(\sigma \cdot D)u \in \mathbf{h}^2),$$

where $\sigma \cdot D := \sum_{j=1}^3 \sigma_j D_j$.

Let

$$J_c^\pm := \left[\lambda \pm mc^2 - \frac{1}{c^\tau}, \lambda \pm mc^2 + \frac{1}{c^\tau}\right],$$
$$I_c^\pm := \left[a \pm mc^2, b \pm mc^2\right],$$

for $0 < \tau < 1$. Then we have

$$E_c(I_c^+ \setminus J_c^+)\, Q_+\Phi \to 0,$$
$$E_c(J_c^+) Q_+\Phi \to E_+(\{\lambda\}) Q_+\Phi$$
$$\left(\textit{or} \begin{array}{l} E_c(I_c^- \setminus J_c^-)\, Q_-\Phi \to 0, \\ E_c(J_c^-) Q_-\Phi \to E_-(\{\lambda\}) Q_-\Phi \end{array} \right)$$

strongly in $\mathcal{H}$ as $c \to \infty$ for any $\Phi \in \mathcal{H}$.

To prove Theorem 2.1 we use a one-parameter unitary group

$$U_s = \exp(-isK), \quad K := \frac{i}{2m}\beta(\alpha \cdot D),$$

which is the first approximation of Foldy-Wouthuysen-Tani transform. The operator K is self-adjoint in $\mathcal{H}$ such that

$$C_0^\infty(\mathbf{R}^3)^4 \subset D(K) \subset H^1_{\mathrm{loc}}(\mathbf{R}^3)^4,$$

where $H^1_{\mathrm{loc}}(\mathbf{R}^3)^4$ is the local Sobolev space.

Let $\Phi \in C_0^\infty(\mathbf{R}^3)^4$. Since $U_s\Phi$ is a solution to the symmetric hyperbolic equation with the finite propagation property, the support of $U_s\Phi$ is also compact. Therefore we have

$$U_s(\alpha \cdot D)U_s^{-1}\Phi = (\alpha \cdot D)U_{-2s}\Phi,$$
$$U_s\beta U_s^{-1}\Phi = \beta U_{-2s}\Phi,$$
$$U_s H_c U_s^{-1}\Phi$$

(3) $$= \left[\frac{1}{s}(\alpha \cdot D) + \frac{m}{s^2}\beta\right] U_{-2s}\Phi + U_s V U_{-s}\Phi,$$

where $s = 1/c$.

Lemma 2.2. *Let $T_s := U_s H_c U_s^{-1}$. For any $\Phi \in C_0^\infty(\mathbf{R}^3)^4$ we have*

$$\left[T_s - \frac{m}{s^2}\beta\right]\Phi = U_s H_c U_s^{-1}\Phi - \frac{m}{s^2}\beta\Phi$$
$$\to \left(\frac{1}{2m}(\alpha \cdot D)^2\beta + V\right)\Phi = S\Phi$$

in $\mathcal{H}$ as $s = 1/c \to 0$.

We sketch the proof of Lemma 2.2. By Maclaurin expansion and (1) we have

$$U_{-2s}\Phi = \Phi - \frac{s}{m}\beta(\alpha \cdot D)\Phi - \frac{s^2}{2m^2}(\alpha \cdot D)^2\Phi + O(s^3).$$

as $s \to 0$. For the first term of (3) we obtain

$$\left[\frac{1}{s}(\alpha \cdot D) + \frac{m}{s^2}\beta\right] U_{-2s}\Phi$$

$$= \frac{1}{2m}(\alpha \cdot D)^2 \beta\Phi + \frac{m}{s^2}\beta\Phi + O(s) \quad (s \to 0).$$

Since the supports of $U_{-s}\Phi$ for $|s| \le 1$ are contained in a ball B_R as remarked above, we obtain, by noting $U_{-s} \to I$ $(s \to 0)$ strongly in $\mathcal{H}$,

$$\begin{aligned} &U_s V U_{-s}\Phi - V\Phi \\ &= U_s V(U_{-s} - I)\Phi + (U_s - I)V\Phi \to 0 \quad \text{in } \mathcal{H}, \end{aligned}$$

which gives Lemma 2.2.

Lemma 2.2 gives the following

Lemma 2.3. *Let $I = [\alpha, \beta]$. Suppose that S_+ (or S_-) on $C_0^\infty(\mathbf{R}^3)^2$ is essentially self-adjoint in $\mathbf{h}^2$, and neither α nor β is an eigenvalue of the self-adjoint extension S_+. Then we have*

$$(4) \qquad E_c([\alpha + mc^2, \beta + mc^2])Q_+\Phi \to E_+(I)Q_+\Phi$$
$$(\textit{or } E_c([\alpha - mc^2, \beta - mc^2])Q_-\Phi \to E_-(I)Q_-\Phi)$$

strongly in $\mathcal{H}$ for every $\Phi \in \mathcal{H}$ as $c \to \infty$.

We outline the proof. Lemma 2.2 and the essential self-adjointness of S_+ yield

$$\left(T_s - \frac{m}{s^2} - z\right)^{-1} Q_+\Phi \to (SQ_+ - z)^{-1}Q_+\Phi$$

strongly in $\mathcal{H}$ as $s = 1/c \to 0$ for every $\Phi \in \mathcal{H}$ and $\operatorname{Im} z \ne 0$. Let $f(\lambda) \in C_0^\infty(\mathbf{R})$. Then we obtain by using Helffer-Sjöstrand's formula (see Helffer-Sjöstrand [5], Isozaki [8])

$$f\left(T_s - \frac{m}{s^2}\right) Q_+\Phi \to f(SQ_+)Q_+\Phi$$

strongly in $\mathcal{H}$. Since $U_s \to I$ strongly and

$$f\left(T_s - \frac{m}{s^2}\right) = U_s f\left(H_c - mc^2\right) U_{-s},$$

we have

$$f\left(H_c - mc^2\right) Q_+\Phi \to f(SQ_+)Q_+\Phi \quad (c \to \infty)$$

strongly in $\mathcal{H}$. The lemma follows by applying the well known approximation argument, see e.g. Theorem VIII.24 in [10].

Let λ be an isolated eigenvalue of S_+ with multiplicity m and

$$\psi_1, \psi_2, \ldots, \psi_m$$

the corresponding orthonormal eigenfunctions of S_+ in $\mathbf{h}^2$. Put

$$\Psi_j(c) := \begin{pmatrix} \psi_j \\ (1/2mc)(\sigma \cdot D)\psi_j \end{pmatrix},$$

$$\Psi_j := \Psi_j(\infty) = \begin{pmatrix} \psi_j \\ \mathbf{0} \end{pmatrix}.$$

Then we have

$$\begin{aligned} &\left(H_c - mc^2\right)\Psi_j(c) - \lambda\Psi_j(c) \\ &= \begin{pmatrix} V_+ - \lambda & c(\sigma \cdot D) \\ c(\sigma \cdot D) & V_- - \lambda - 2mc^2 \end{pmatrix} \Psi_j(c) \\ &= \frac{1}{2mc} \begin{pmatrix} \mathbf{0} \\ (V_- - \lambda)(\sigma \cdot D)\psi_j \end{pmatrix} = O\left(\frac{1}{c}\right). \end{aligned}$$

Here we used the assumption that $(\sigma \cdot D)u$ and $V_-(\sigma \cdot D)u \in \mathbf{h}^2$. Thus we obtain the first statement of the following lemma.

Lemma 2.4. *Suppose the conditions in* Theorem 2.1. *Let $\psi_j, \Psi_j(c), \Psi$ be as above, and let $P := E_+(\{\lambda\})$, that is,*

$$P\Phi = \sum_{j=1}^m \langle \Phi, \Psi_j \rangle \Psi_j \quad (\Phi \in \mathcal{H}).$$

Let P_c be the orthogonal projection on the subspace spanned by $\{\Psi_j(c)\}_{j=1,2,\ldots,m}$. Then we have

$$(5) \qquad \left\|\left(I - E_c\left(J_c^+\right)\right)\Psi_j(c)\right\| = O(c^{\tau-1}),$$

$$(6) \qquad \left(I - E_c\left(J_c^+\right)\right) P_c\Phi \to 0,$$

$$(7) \qquad P_c\Phi \to P\Phi,$$

$$(8) \qquad E_c\left(I_c^+\right) Q_+\Phi \to P\Phi,$$

strongly in $\mathcal{H}$ as $c \to \infty$ for every $\Phi \in \mathcal{H}$.

The relation (6) is a consequence of (5). The property (7) is obvious, and (8) follows from (4) in Lemma 2.3.

Proof of Theorem 2.1. The above (7) and (8) yield

$$\begin{aligned} &\|E_c(J_c^+)(I - P_c)Q_+\Phi\| \\ &\le \|E_c(J_c^+)(I - P)Q_+\Phi\| \\ &\quad + \|E_c(J_c^+)(P - P_c)Q_+\Phi\| \\ &\le \|E_c(I_c^+)Q_+(I - P)\Phi\| + \|(P - P_c)Q_+\Phi\| \\ &\quad \to 0 \quad (c \to \infty), \end{aligned}$$

which together with (6) and (7) gives

$$\begin{aligned} &E_c(J_c^+)Q_+\Phi - P\Phi \\ &= E_c(J_c^+)(I - P_c)Q_+\Phi - (I - E_c(J_c^+))P_cQ_+\Phi \\ &\quad + P_cQ_+\Phi - P\Phi \to 0. \end{aligned}$$

Consequently, we have from (8)

$$\begin{aligned} &E_c\left(I_c^+ \setminus J_s^+\right) Q_+\Phi \\ &= E_c\left(I_c^+\right) Q_+\Phi - E_c\left(J_s^+\right) Q_+\Phi \\ &\to 0, \end{aligned}$$

which completes the proof. □

3. An application to potentials diverging at infinity. We apply Theorem 2.1 to the case when V is scalar and diverges to infinity as $|x| \to \infty$.

If $b_j(x) \in C^1$ and $v(x) \in C^0$ satisfies

$$v(x) \geq -C_1 - C_2|x|^2 \quad (C_1, C_2 > 0),$$

S_+ on $C_0^\infty(\mathbf{R}^3)$ is essentially self-adjoint in $\mathbf{h}^2$. This fact can be shown along the lines of Ikebe-Kato [7].

It can be shown by Rellich's criterion (e.g., Reed-Simon [11, Theorem XIII.65]) that, if we assume

$$(9) \qquad v(x) \to +\infty \quad (|x| \to \infty),$$

the spectrum of S_+ is purely discrete, that is, the spectrum $\sigma(S_+)$ consists of discrete eigenvalues with finite multiplicity. As an application of Theorem 2.1 we give the following

Theorem 3.1. *Assume that each $b_j(x) \in C^3$, and $v(x) \in C^1(\mathbf{R}^3)$ satisfies* (9) *and*

$$(10) \qquad |(\nabla v)(x)| = o(v(x)^{3/2}) \quad (|x| \to \infty).$$

Let

$$\lambda_1 < \lambda_2 < \cdots \lambda_n < \cdots \to +\infty \quad (n \to \infty)$$

be the discrete eigenvalues of S_+. Fix an eigenvalue λ_N. Let us take any interval $I = (a, b) \ni \lambda_N$ such that $\overline{I} \subset (\lambda_{N-1}, \lambda_{N+1})$, and I_c^+, J_c^+ as in Theorem 2.1. *Then we have*

$$E_c(I_c^+ \setminus J_c^+)Q_+\Phi \to 0,$$
$$E_c(J_c^+)Q_+\Phi \to E_+(\{\lambda_N\})Q_+\Phi$$

strongly in $\mathcal{H}$ as $c \to \infty$ for any $\Phi \in \mathcal{H}$.

It suffices to show (iii) among the assumptions in Theorem 2.1. To this end we give the following lemma.

Lemma 3.2. *Assume $b_j(x) \in C^1$, $v(x) \in C^1(\mathbf{R}^3)$ with* (9) *and* (10). *Suppose that λ is an eigenvalue of S_+, and $u(x) \in D(S_+)$ satisfies $S_+u = \lambda u$. Then we have*

$$(11) \qquad \int_{\mathbf{R}^3} v^2 \left[\frac{|(\sigma \cdot D)u|^2}{2m} + v|u|^2\right] dx < \infty.$$

Sketch of the proof. Since $u \in D(S_+)$ satisfies

$$(12) \qquad \frac{1}{2m}(\sigma \cdot D)^2 u + vu = \lambda u,$$

we obtain

$$\int_{\mathbf{R}^3} \left[\frac{|(\sigma \cdot D)u|^2}{2m} + v|u|^2\right] dx < \infty.$$

In view of (9) there is a large number R_0 such that $v(x) > 0$ for $|x| \geq R_0$. We shall prove

$$(13) \qquad \int_{|x|\geq R_0} v^{n/2} \left[\frac{|(\sigma \cdot D)u|^2}{2m} + v|u|^2\right] dx < \infty,$$

for $n = 0, 1, 2, \ldots$, inductively. Assume (13) for n. Integrating the inner product of (12) and $v^{(n+1)/2}u$ over $B(R_1, R) := \{x \mid R_1 \leq |x| \leq R\}$, we have

$$\begin{aligned}
&\int_{B(R_1,R)} v^{(n+1)/2} \left[\frac{|(\sigma \cdot D)u|^2}{2m} + v|u|^2\right] dx \\
&- \lambda \int_{B(R_1,R)} v^{(n+1)/2}|u|^2 dx \\
&= \left[\int_{|x|=R} - \int_{|x|=R_1}\right] \frac{v^{(n+1)/2}}{2m} \\
&\quad \times \sum_{j=1}^{3} \frac{x_j}{|x|} \langle i\sigma_j(\sigma \cdot D)u, u\rangle\, dS \\
&\quad - \frac{n+1}{4m} \int_{B(R_1,R)} v^{(n-1)/2} \sum_{j=1}^{3} \frac{\partial v}{\partial x_j} \langle i\sigma_j(\sigma \cdot D)u, u\rangle\, dx
\end{aligned}$$

for any $R_0 < R_1 < R$. Now, (13) gives

$$\begin{aligned}
&\liminf_{R\to\infty} \left|\int_{|x|=R} v^{(n+1)/2} \sum_{j=1}^{3} \frac{x_j}{|x|} \langle \sigma_j(\sigma \cdot D)u, u\rangle\, dS\right| \\
&\leq \liminf_{R\to\infty} \int_{|x|=R} v^{n/2} \left[|(\sigma \cdot D)u|^2 + v|u|^2\right] dS = 0.
\end{aligned}$$

The assumptions (9) and (10) imply, for a sufficiently large R_1,

$$\begin{aligned}
&\frac{n+1}{4m} \left|v^{(n-1)/2} \sum_{j=1}^{3} \frac{\partial v}{\partial x_j} \langle \sigma_j(\sigma \cdot D)u, u\rangle\right| \\
&\leq \frac{1}{2} v^{(n+1)/2} \left[\frac{|(\sigma \cdot D)u|^2}{2m} + v|u|^2\right]
\end{aligned}$$

for $|x| \geq R_1$. Thus we have

$$\begin{aligned}
&\frac{1}{2} \int_{|x|\geq R_1} v^{(n+1)/2} \left[\frac{|(\sigma \cdot D)u|^2}{2m} + v|u|^2\right] dx \\
&\leq \int_{|x|=R_1} \frac{v^{(n+1)/2}}{2m} \left|\sum_{j=1}^{3} \frac{x_j}{|x|} \langle \sigma_j(\sigma \cdot D)u, u\rangle\right| dS \\
&\quad + |\lambda| \int_{|x|\geq R_1} (1 + v^{(n+2)/2})|u|^2\, dx
\end{aligned}$$

which yields (13) for $n + 1$. □

Remark 3.3. The property (13) is closely related to the exponential decay of eigenfunctions of Schrödinger equations (cf. Agmon [1], Shen [13]).

The condition (10) is satisfied by a large class of potentials $v(x)$ with (9) such as $v(x) = \exp(|x|^2)$, $v(x) = \exp[\exp(|x|^2)]$.

Remark 3.4. If $v(x) = O(|x|^2)$ at infinity with (9) and $b_j(x) \equiv 0$ $(1 \leq j \leq 3)$,

$$S_- = \frac{1}{2m}\Delta + v(x)$$

on $C_0^\infty(\mathbf{R}^3)^2$ is essentially self-adjoint in $\mathbf{h}^2$ as stated at the beginning of this section. In this case both $\sigma(H_c)$ and $\sigma(S_-)$ have purely continuous spectrum, which coincides with the whole real line $\mathbf{R}$ under some additional conditions (see, e.g., Kalf-Ōkaji-Yamada [9], Uchiyama-Yamada [15]). Then Lemma 2.3 implies, for any interval $[a, b]$,

$$E_c(I_c^-)Q_-\Phi \to E_-(I)Q_-\Phi$$

strongly in $\mathcal{H}$ for every $\Phi \in \mathcal{H}$ as $c \to \infty$.

Remark 3.5. If $V(x) = v(x)\beta$, that is,

$$V_+(x) = -V_-(x) = v(x)I_2, \quad S_- = -S_+$$

with (9) and (10), not only $S_\pm$ but also H_c is purely discrete (e.g., Yamada [18]). Then the results as in Theorem 3.1 are valid for both S_+ and S_-.

Acknowledgements. This work was partially supported by Open Research Center Project for Private Universities: matching fund subsidy from MEXT, 2004–2008.

The authors express their gratitude to the referee for valuable advices.

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