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An iterative approach to monochromatic phaseless inverse scattering

A. D. Agaltsov¹, T. Hohage², R. G. Novikov³

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Abstract

This paper is concerned with the inverse problem to recover a compactly supported Schrödinger potential given the differential scattering cross section, i.e. the modulus, but not the phase of the scattering amplitude. To compensate for the missing phase information we assume additional measurements of the differential cross section in the presence of known background objects. We propose an iterative scheme for the numerical solution of this problem and prove that it converges globally of arbitrarily high order depending on the smoothness of the unknown potential as the energy tends to infinity. At fixed energy, however, the proposed iteration does not converge to the true solution even for exact data. Nevertheless, numerical experiments show that it yields remarkably accurate approximations with small computational effort even for moderate energies. At small noise levels it may be worth to improve these approximations by a few steps of a locally convergent iterative regularization method, and we demonstrate to which extent this reduces the reconstruction error.

Keywords: Inverse scattering problems, phaseless inverse scattering, Schrödinger equation

AMS subject classification: 35J10, 35R30, 65N21, 81U40, 78A46

1 Introduction

In quantum mechanics the interaction of an elementary particle at fixed energy $E > 0$ with a macroscopic object contained in a bounded domain D is described by the Schrödinger equation

$$-\Delta\psi + v(x)\psi = E\psi, \quad x \in \mathbb{R}^d. \quad (1.1a)$$

Here Δ is the standard Laplacian in x , and the potential function v is assumed to satisfy

$$v \in L^\infty(\mathbb{R}^d), \quad \text{supp } v \subset D \subset \mathbb{R}^d, \quad d \geq 2. \quad (1.1b)$$

Equation (1.1a) can be also considered as the Helmholtz equation of acoustic and electrodynamic wave propagation at fixed frequency.

For equation (1.1a) we consider the classical scattering solutions $\psi^+(\cdot, k)$ of the form $\psi^+(x, k) = e^{ikx} + \psi^s(x, k)$ with a plane incident field e^{ikx} such that $k \in \mathbb{R}^d$, $|k|^2 = E$, and a scattered field $\psi^s(\cdot, k)$ satisfying the Sommerfeld radiation condition

$$|x|^{\frac{d-1}{2}} \left(\frac{\partial}{\partial|x|} - i|k| \right) \psi^s(x, k) \rightarrow 0 \quad \text{as } |x| \rightarrow \infty \quad (1.1c)$$

uniformly in $x/|x|$. This implies that ψ^s has the asymptotic behavior

$$\begin{aligned} \psi^s(x, k) &= c(d, |k|) \frac{e^{i|k||x|}}{|x|^{\frac{d-1}{2}}} f_E \left(k, |k| \frac{x}{|x|} \right) + \mathcal{O} \left(|x|^{-\frac{d+1}{2}} \right), \quad |x| \rightarrow \infty, \\ c(d, |k|) &:= -\pi i (-2\pi i)^{(d-1)/2} |k|^{(d-3)/2} \end{aligned} \quad (1.2)$$

¹Max-Planck Institute for Solar Systems Research, Justus-von-Liebig-Weg 3, 37077 Göttingen, Germany (agaltsov@mps.mpg.de).

²Institute for Numerical and Applied Mathematics, University of Göttingen, Lotzestr. 16-18, 37083 Göttingen, Germany (hohage@math.uni-goettingen.de) and Max-Planck Institute for Solar Systems Research.

³CMAP, Ecole Polytechnique, CNRS, Université Paris-Saclay, 91128 Palaiseau, France; and IEPT RAS, 117997 Moscow, Russia (novikov@cmap.polytechnique.fr).

with a function f_E called the scattering amplitude or far field pattern at energy E . There are different conventions for the choice of the constant $c(d, |k|)$. The one above leads to the following simple asymptotic relation between the scattering amplitude and the inverse Fourier transform of v , see, e.g., [9, 28]:

$$\widehat{v}(k-l) = f_E(k, l) + \mathcal{O}(E^{-\frac{1}{2}}), \quad E \rightarrow +\infty, \quad (1.3)$$

$$\widehat{v}(p) := (2\pi)^{-d} \int_{\mathbb{R}^d} e^{ipx} v(x) dx, \quad p \in \mathbb{R}^d \quad (1.4)$$

$|f_E(k, l)|^2$ is known as the differential scattering cross section for equation (1.1a). In quantum mechanics this quantity describes the probability density of scattering of particle with initial impulse k into direction $l/|l| \neq k/|k|$, see, for example, [10, Chapter 1, Section 6]. Typically, the differential cross section is the only measurable quantity whereas the phase of the scattering amplitude cannot be determined directly by physical experiments. The problem of finding v from $|f_E|^2$ is known as the phaseless inverse scattering problem for equation (1.1a). Whereas the inverse scattering problem with phase information for equation (1.1a), i.e. the problem of finding v from f_E , has been studied intensively for a long time (see [4, 5, 6, 7, 8, 9, 12, 13, 18, 17, 22, 23, 24, 25, 28] and references therein), much less studies were performed in the phaseless case (see [1, 7, 20, 21, 30, 26, 27, 29]).

It is well known that the phaseless scattering data $|f_E|^2$ does not determine v uniquely even if $|f_E|^2$ is given completely for all $E > 0$; see, e.g., [29]. In the present work we continue studies of [29, 1] assuming additional measurements of the following form: For the unknown v satisfying (1.1b) we consider additional a priori known background scatterers w_1, \dots, w_L such that

$$\begin{aligned} w_l &\in L^\infty(\mathbb{R}^d), \quad \text{supp } w_l \subset \Omega_l, \\ \Omega_l &\text{ is an open bounded domain in } \mathbb{R}^d, \\ w_l &\neq 0, \quad w_l \neq w_{\tilde{l}} \text{ if } l \neq \tilde{l} \text{ (in } L^\infty(\mathbb{R}^d)), \end{aligned} \quad (1.5)$$

where $l, \tilde{l} \in \{1, \dots, L\}$. In practice, we also typically have

$$\Omega_l \cap D = \emptyset,$$

but this property will not be needed in our analysis. We set

$$S = \{|f_E|^2, |f_{E,1}|^2, \dots, |f_{E,L}|^2\}, \quad (1.6)$$

where f_E is the scattering amplitude for v at energy E , and $f_{E,1}, \dots, f_{E,L}$ are the scattering amplitudes for v_1, \dots, v_L , where

$$v_l = v + w_l, \quad l = 1, \dots, L. \quad (1.7)$$

One can see that S consists of the phaseless scattering data $|f_E|^2, |f_{E,1}|^2, \dots, |f_{E,L}|^2$ measured sequentially, first, for the unknown scatterer v and then for the unknown scatterer v in the presence of known scatterer w_l disjoint from v for $l = 1, \dots, L$. We consider the following inverse scattering problem without phase information for equation (1.1a):

Problem 1. *Reconstruct coefficient v from the phaseless scattering data S for some appropriate background scatterers w_1, \dots, w_L .*

In this paper we propose an iterative approach to Problem 1 with iterates $u_E^{(j)}$, $j = 1, 2, \dots$ and prove error bounds of the form

$$\|u_E^{(j)} - v\|_{L^\infty} = \mathcal{O}(E^{-\alpha_j}) \quad (1.8)$$

with exponents α_j tending to ∞ as $j \rightarrow \infty$ for infinitely smooth potentials v .

For the inverse scattering problem with phase information such a substantial improvement of the Born approximation, which serve as first iterate u_1 (see (1.3)) has been obtained in [28], and first numerical tests were reported in [5].

Studies on Problem 1 in dimension $d = 1$ for $L = 1$ were started in [3], where phaseless scattering data was considered for all $E > 0$. Note also that a phaseless optical imaging in the presence of known background objects was considered, in particular, in [11]. Studies on Problem 1 in dimension $d \geq 2$ were started in [29] and continued recently in [1]. The key result of [29] consists in a proper extension of formula (1.3) for the Fourier transform \hat{v} of v to the phaseless case of Problem 1, $d \geq 2$, which will be detailed in Section 3.1. The main results of [1] consist in proper extensions of formula (2.8) in the configuration space to the case of Problem 1 for $d \geq 2$; see also Section 3.1. However, the convergence of the approximations to v as $E \rightarrow +\infty$ in [1] is slow, in particular, the exponent α in (1.8) is always $\leq \frac{1}{2}$.

In addition, our theoretical iterative monochromatic reconstructions for Problem 1 are illustrated numerically in Section 4.

2 Iterative inversion with phase information

2.1 Inverse scattering with phase information

Recall that the scattering amplitude f_E is defined on the set

$$\mathcal{M}_E = \{(k, l) \in \mathbb{R}^d \times \mathbb{R}^d : |k|^2 = |l|^2 = E\}. \quad (2.1)$$

In view of (1.3) we assume that the scattering amplitude, and later the differential cross section is defined on some subset $\mathcal{M}_E^m \subset \mathcal{M}_E$ such that the function

$$\tilde{\Phi} : \mathcal{M}_E^m \rightarrow \mathcal{B}_{2\sqrt{E}}^d \quad \tilde{\Phi}(k, l) := k - l \quad (2.2)$$

is surjective. Here and in the following \mathcal{B}_r^d denotes the closed ball

$$\mathcal{B}_r^d = \{p \in \mathbb{R}^d : |p| \leq r\}, \quad r > 0. \quad (2.3)$$

For $d \geq 2$ we may construct a d -dimensional subset $\mathcal{M}_E^m \subset \mathcal{M}_E$ such that $\tilde{\Phi}$ is bijective as follows: Let us choose a piece-wise continuous function $\gamma : \mathcal{B}_{2\sqrt{E}}^d \rightarrow \mathbb{R}^d$ such that $|\gamma(p)| = 1$ and $\gamma(p)p = 0$ for all $p \in \mathcal{B}_{2\sqrt{E}}^d$ and set

$$\mathcal{M}_E^m = \left\{ \left(\frac{p}{2} + \left(E - \frac{p^2}{4}\right)^{1/2} \gamma(p), -\frac{p}{2} + \left(E - \frac{p^2}{4}\right)^{1/2} \gamma(p) \right) : p \in \mathcal{B}_{2\sqrt{E}}^d \right\}. \quad (2.4)$$

To use the Born approximation (1.3) and its refinements if $\tilde{\Phi}$ is not injective, we average over the set $\tilde{\Phi}^{-1}(p)$. To this end we assume that for all $p \in \mathcal{B}_{2\sqrt{E}}^d$ the set $\tilde{\Phi}^{-1}(p)$ is a piecewise smooth manifold of size $|\tilde{\Phi}^{-1}(p)|$ and define the averaging operator

$$\Phi : L^1(\mathcal{M}_E^m) \rightarrow L^1(\mathcal{B}_{2\sqrt{E}}^d), \quad (\Phi f)(p) := \frac{1}{|\tilde{\Phi}^{-1}(p)|} \int_{\tilde{\Phi}^{-1}(p)} f_E(k, l) d(k, l). \quad (2.5)$$

Using this mapping we can define an approximation u_E to v on D by

$$u_E(x) := \int_{\mathcal{B}_{2\sqrt{E}}^d} e^{-ipx} (\Phi f)(p) dp, \quad x \in D. \quad (2.6)$$

Let $W^{n,1}(\mathbb{R}^d)$ denote the Sobolev space of n -times smooth functions in the sense of $L^1(\mathbb{R}^d)$:

$$W^{n,1}(\mathbb{R}^d) := \{u \in L^1(\mathbb{R}^d) : \|u\|_{n,1} < \infty\} \quad \text{with} \quad (2.7)$$

$$\|u\|_{n,1} := \max_{|J| \leq n} \left\| \frac{\partial^{|J|} u}{\partial x^J} \right\|_{L^1(\mathbb{R}^d)}, \quad n \in \mathbb{N} \cup \{0\}.$$

If $v \in W^{n,1}(\mathbb{R}^d)$, $n > d$, in addition to the initial assumptions (1.1b), then u_E satisfies the error bound

$$\|u_E - v\|_{L^\infty(D)} = \mathcal{O}(E^{-\alpha}) \quad \text{as } E \rightarrow +\infty \quad \text{with } \alpha = \frac{n-d}{2n} \quad (2.8)$$

for $d \geq 2$; see, for example, [28]. Essential improvements of the approximation u_E in (2.6) were achieved in [23, 24, 28]. In particular, formula (2.8) was principally improved in [28] by constructing iteratively nonlinear approximate reconstructions $u_E^{(j)}$ such that $u_E^{(1)} = u_E$ and

$$\|u_E^{(j)} - v\|_{L^\infty(D)} = \mathcal{O}(E^{-\alpha_j}) \quad \text{with } \alpha_j = \frac{n-d}{2d} \left(1 - \left(\frac{n-d}{n}\right)^j\right), \quad j \geq 1, \quad (2.9)$$

as $E \rightarrow +\infty$ for $d \geq 2$ if $v \in W^{n,1}(\mathbb{R}^d)$, $n > d$, in addition to the initial assumptions (1.1b). The point is that

$$\begin{aligned} \alpha_j &\rightarrow \alpha_\infty = \frac{n-d}{2d} && \text{as } j \rightarrow +\infty, \\ \alpha_j &\rightarrow \frac{j}{2} && \text{as } n \rightarrow +\infty, \\ \alpha_\infty &\rightarrow +\infty && \text{as } n \rightarrow +\infty; \end{aligned} \quad (2.10)$$

that is the convergence in (2.9) as $E \rightarrow +\infty$ is drastically better than the convergence in (2.8), at least, for large n and j .

2.2 Iterative step for phased inverse scattering

Recall that the outgoing fundamental solution to the Helmholtz equation is given by

$$G^+(x, k) = -(2\pi)^{-d} \int_{\mathbb{R}^d} \frac{e^{i\xi x} d\xi}{\xi^2 - k^2 - i0} = \frac{i}{4} \left(\frac{k}{2\pi|x-y|}\right)^\nu H_\nu^{(1)}(k|x-y|) \quad \text{with } \nu := \frac{d}{2} - 1,$$

where $H_\nu^{(1)}$ denotes the Hankel function of the first kind of order ν . Let $\mathcal{G}^+(k)$ denote the convolution operator with kernel $G^+(\cdot, k)$. The following estimate, which goes back to [2], is essential for studies on direct scattering (see, e.g., [8] (§29), [28], and references therein) and will also be crucial for our analysis:

$$\begin{aligned} \|\Lambda^{-s} \mathcal{G}^+(k) \Lambda^{-s}\|_{L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)} &\leq a_0(d, s) |k|^{-1}, \\ k \in \mathbb{R}^d, |k| &\geq 1, \quad \text{for } s > \frac{1}{2}. \end{aligned} \quad (2.11)$$

Here Λ^{-s} denotes the operator of multiplication by $(1 + |x|^2)^{-s/2}$.

Let v , satisfying (1.1b), be the unknown potential and v_E^* be an approximation to v , and assume that there exist constants $A, E^*, K, \alpha > 0$ such that

$$v_E^* \in L^\infty(\mathbb{R}^d), \quad \text{supp } v_E^* \subset D \quad (2.12a)$$

$$\|v_E^* - v\|_{L^\infty(D)} \leq AE^{-\alpha} \quad (2.12b)$$

$$\|v\|_{L^\infty(\mathbb{R}^d)} \leq K, \quad \|v_E^*\|_{L^\infty(\mathbb{R}^d)} \leq K \quad (2.12c)$$

for all $E \geq E^*$.

For inverse scattering with phase information the iterative step of [28] is based on the following lemma.

Lemma 2.1. *Let v , satisfying (1.1b), be the unknown potential and $v^*(\cdot, E)$ be an approximation to v satisfying (2.12) for some $A > 0$, $\alpha \geq 0$, $K > 0$ and $E^* = E^*(K, D)$, where*

$$E^*(K, D) = 2Ka_0(d, s) \sup_{x \in D} (1 + |x|^2)^{s/2}, \quad (2.13)$$

for some $s > \frac{1}{2}$, where $a_0(d, s)$ is the constant of (2.11).

Let f_E, f_E^* be the scattering amplitudes of v, v_E^* . Then there exists a constant $\mu_{1,\S 2.2} = \mu_{1,\S 2.2}(A, K, D) > 0$ such that

$$\sup_{(k,l) \in \mathcal{M}_E} |f_E(k,l) - f_E^*(k,l) + \widehat{v_E^*}(k-l) - \widehat{v}(k-l)| \leq \mu_{1,\S 2.2} E^{-\alpha - \frac{1}{2}}, \quad E \geq E^*, \quad (2.14)$$

where $\widehat{v}, \widehat{v_E^*}$ are the Fourier transforms of v, v_E^* defined according to (1.4).

Note that in this paper we use the notation $\mu_{k,\S X}, k \geq 1$, for the constants of Section X.

Lemma 2.1 follows from Lemma 3.2 of [28] for $v_0 \equiv 0$, where v_0 is the background potential of [28]. The proof of Lemma 3.2 of [28] essentially uses estimate (2.11).

In particular, due to (2.14), the function

$$U_E^{**} := \Phi f_E - \Phi f_E^* + \widehat{v_E^*}, \quad (2.15)$$

where $\Phi f_E, \Phi f_E^*$ are defined according to (2.5), satisfies the following improved error estimate compared to (2.12b):

$$\|U_E^{**} - \widehat{v}\|_{L^\infty(\mathcal{B}_{2\sqrt{E}}^d)} \leq \mu_{1,\S 2.2} E^{-\alpha - \frac{1}{2}}, \quad E \geq E^*. \quad (2.16)$$

If $v \in W^{n,1}(\mathbb{R}^d)$, $n > d$ (in addition to the initial assumptions (1.1b)), and if

$$\alpha < \frac{n}{2d} - \frac{1}{2}, \quad (2.17)$$

then this permits to construct an improved approximation v_E^{**} to the unknown potential v as follows:

$$v_E^{**}(x) := \begin{cases} \int_{\mathcal{B}_{r(E)}^d} e^{-ipx} U_E^{**}(p) dp, & x \in D, \\ 0, & x \notin D, \end{cases} \quad r(E) := 2\tau E^{\frac{1+2\alpha}{2n}}, \quad \tau \in (0, 1], \quad (2.18)$$

Here U_E^{**} is defined in (2.15) and $E^* = E^*(K, D)$ is the constant of (2.13). It follows that there exists a constant $B > 0$ such that

$$\|v_E^{**} - v\|_{L^\infty(D)} \leq B E^{-\beta}, \quad E \geq E^* \text{ with } \beta := \alpha(1 - \frac{d}{n}) + \frac{1}{2} - \frac{d}{2n}, \quad (2.19)$$

Note that

$$\alpha < \beta < \frac{n}{2d} - \frac{1}{2}$$

and that condition (2.17) implies that $r(E) \leq 2\sqrt{E}$, so that the definition (2.18) is correct.

3 Iterative inversion from phaseless data

3.1 Low order potential reconstruction formulas from phaseless data

In this subsection we extend the formulas (1.3) and (2.8) to the phaseless case. The key result of [29] consists in the following formulas for solving Problem 1 in dimension $d \geq 2$ for $L = 2$ at high energies E :

$$\sup_{p \in \mathcal{B}_{2\sqrt{E}}^d} \left| |\widehat{v}_l(p)|^2 - |\Phi f_{E,l}(p)|^2 \right| = \mathcal{O}(E^{-\frac{1}{2}}), \quad E \rightarrow +\infty, \quad l = 0, 1, 2, \quad (3.1)$$

where $v_0 = v$, v_l is defined by (1.7), $l = 1, 2$, $f_{E,0} = f_E, f_{E,1}, f_{E,2}$ are the scattering amplitudes for v_0, v_1, v_2 , respectively; in addition,

$$\begin{pmatrix} \operatorname{Re} \widehat{v} \\ \operatorname{Im} \widehat{v} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \operatorname{Re} \widehat{w}_1 & \operatorname{Im} \widehat{w}_1 \\ \operatorname{Re} \widehat{w}_2 & \operatorname{Im} \widehat{w}_2 \end{pmatrix}^{-1} \begin{pmatrix} |\widehat{v}_1|^2 - |\widehat{v}|^2 - |\widehat{w}_1|^2 \\ |\widehat{v}_2|^2 - |\widehat{v}|^2 - |\widehat{w}_2|^2 \end{pmatrix}, \quad (3.2)$$

where $\widehat{v} = \widehat{v}(p)$, $\widehat{v}_l = \widehat{v}_l(p)$, $\widehat{w}_l = \widehat{w}_l(p)$, $p \in \mathbb{R}^d$, and formula (3.2) is considered for all p such that the determinant

$$\zeta_{\widehat{w}_1, \widehat{w}_2}(p) := \operatorname{Re} \widehat{w}_1(p) \operatorname{Im} \widehat{w}_2(p) - \operatorname{Im} \widehat{w}_1(p) \operatorname{Re} \widehat{w}_2(p) \neq 0. \quad (3.3)$$

Formulas (3.1), (3.2) can be considered as a natural extension of formula (1.3) to the phaseless case of Problem 1, $d \geq 2$, $L = 2$ and lead to the function Urec defined in Algorithm 1 for the approximate reconstruction $U_{\widehat{w}_1, \widehat{w}_2}$ of \widehat{v} :

$$U_{\widehat{w}_1, \widehat{w}_2}(p) := \operatorname{Urec}(\widehat{w}_1(p), \widehat{w}_2(p), \Phi|f_E|^2(p), \Phi|f_{E,1}|^2(p), \Phi|f_{E,2}|^2(p)), \quad |p| \leq 2\sqrt{E} \quad (3.4)$$

Algorithm 1 function $U = \operatorname{Urec}(W_1, W_2, F, F_1, F_2)$

data: Fourier transforms of reference potentials at some point p : $W_1 = \widehat{w}_1(p)$, $W_2 = \widehat{w}_2(p)$;

scattering amplitude at (k, l) , $k - l = p$ without reference potential: $F = |f(k, l)|^2$

scattering amplitudes with reference potentials: $F_1 = |f_1(k, l)|^2$, $F_2 = |f_2(k, l)|^2$

result: approximation to the Fourier transform of the unknown potential v at p : $U \approx \widehat{v}(p)$

$$M := \begin{pmatrix} \operatorname{Re} W_1 & \operatorname{Im} W_1 \\ \operatorname{Re} W_2 & \operatorname{Im} W_2 \end{pmatrix}; \quad b := \begin{pmatrix} F_1 - F - |W_1|^2 \\ F_2 - F - |W_2|^2 \end{pmatrix}; \quad \begin{pmatrix} x \\ y \end{pmatrix} := \frac{1}{2} M^{-1} b; \quad U := x + iy$$

On the level of analysis (e.g., error estimates), the principal complication of (3.1), (3.2) in comparison with (1.3) consists in possible zeros of the determinant $\zeta_{\widehat{w}_1, \widehat{w}_2}$ of (3.3). This complication is, in particular, essential if one tries to transform (3.1), (3.2) into an approximate reconstruction in the configuration space, applying the inverse Fourier transform to $\widehat{v} = \operatorname{Re} \widehat{v} + i \operatorname{Im} \widehat{v}$ of (3.2). For some simplest cases, the results of transforming (3.1), (3.2) to approximate reconstructions in the configuration space, including error estimates, were given in [1].

Background potentials of type A: The first simplest case analyzed in [1] is

$$w_1(x) := w(x - T_1), \quad w_2(x) := iw(x - T_1), \quad x \in \mathbb{R}^d, \quad (3.5)$$

$$\text{for some } w \in C(\mathbb{R}^d) \text{ such that } w = \overline{w}, \quad w(x) = 0 \text{ for } |x| > R, \text{ and} \quad (3.6)$$

$$\widehat{w}(p) = \overline{\widehat{w}(p)} \geq \mu_{1, \S 3.1} (1 + |p|)^{-\sigma}, \quad p \in \mathbb{R}^d,$$

for some fixed $T_1 \in \mathbb{R}^d$, $R > 0$, $\mu_{1, \S 3.1} > 0$, $\sigma > d$, where T_1 and R are chosen in such a way that w_1 satisfies (1.5) (and, as a corollary, w_1, w_2 satisfy (1.5) with $\Omega_2 = \Omega_1$). In addition, a broad class of w satisfying (3.6) was constructed in Lemma 1 of [1]. One can see that

$$\zeta_{\widehat{w}_1, \widehat{w}_2}(p) = |\widehat{w}(p)|^2 \geq \mu_{1, \S 3.1}^2 (1 + |p|)^{-2\sigma}, \quad p \in \mathbb{R}^d, \quad (3.7)$$

if w_1, w_2 are defined by (3.5), (3.6).

Background potentials of type B: The second simplest case analyzed in [1] is

$$w_1(x) = w(x - T_1), \quad w_2(x) = w(x - T_2), \quad x \in \mathbb{R}^d, \quad (3.8)$$

$$\text{for some fixed } T_1, T_2 \in \mathbb{R}^d,$$

where w is the same as in (3.6), and T_1, T_2, R are chosen in such a way that w_1, w_2 satisfy (1.5). One can see that

$$\zeta_{\widehat{w}_1, \widehat{w}_2}(p) = \sin(py) |\widehat{w}(p)|^2, \quad y = T_2 - T_1 \neq 0, \quad p \in \mathbb{R}^d, \quad (3.9)$$

$$|\zeta_{\widehat{w}_1, \widehat{w}_2}(p)| \geq \mu_{1, \S 3.1}^2 (1 + |p|)^{-2\sigma} \frac{2\varepsilon}{\pi}, \quad p \in \mathbb{R}^d \setminus Z_y^\varepsilon,$$

if w_1, w_2 are defined by (3.6), (3.8),

where

$$Z_y^\varepsilon = \{p \in \mathbb{R}^d : py \in (-\varepsilon, \varepsilon) + \pi\mathbb{Z}\}, \quad y \in \mathbb{R}^d \setminus 0, \quad 0 < \varepsilon < 1. \quad (3.10)$$

First consider background potentials w_1, w_2 of type A (see (3.5), (3.6)) and assume that v satisfies (1.1b), $v \in W^{n,1}(\mathbb{R}^d)$ for some $n > d$. Then the result of transforming $U_{\widehat{w}_1, \widehat{w}_2}$ in (3.4) by

$$\begin{aligned} u_E(x) &:= \int_{\mathcal{B}_{r(E)}^d} e^{-ipx} U_{\widehat{w}_1, \widehat{w}_2}(p, E) dp, \quad x \in \mathbb{R}^d, \\ r(E) &= 2\tau E^{\frac{\alpha}{n-d}} \quad \text{for some fixed } \tau \in (0, 1], \end{aligned} \quad (3.11)$$

to an approximate reconstruction in the configuration space is as follows (see [1, Theorem 1]):

$$\|u_E - v\|_{L^\infty(\mathbb{R}^d)} = \mathcal{O}(E^{-\alpha}) \quad E \rightarrow +\infty \quad \text{with } \alpha = \frac{\frac{1}{2}(n-d)}{n+\sigma}. \quad (3.12)$$

Now consider background potentials w_1, w_2 of type B (see (3.8)) and assume again that v satisfies (1.1b), $v \in W^{n,1}(\mathbb{R}^d)$ for some $n > d$. We transform $U_{\widehat{w}_1, \widehat{w}_2}$ in (3.4) to an approximation u_E in the configuration space as follows:

$$\begin{aligned} u_E(x) &= u_{E,1}(x) + u_{E,2}(x), \quad x \in \mathbb{R}^d, \\ u_{E,1}(x) &= \int_{\mathcal{B}_{r(E)}^d \setminus Z_y^\varepsilon(E)} e^{-ipx} U_{\widehat{w}_1, \widehat{w}_2}(p, E) dp, \\ u_{E,2}(x) &= \int_{\mathcal{B}_{r(E)}^d \cap Z_y^\varepsilon(E)} e^{-ipx} U_{\widehat{w}_1, \widehat{w}_2}^\varepsilon(p, E) dp, \\ r(E) &= 2\tau E^{\frac{\alpha}{n-d}}, \quad \varepsilon(E) = E^{-\frac{\alpha}{2}} \quad \text{for some } \tau \in (0, 1], \end{aligned} \quad (3.13)$$

Z_y^ε is defined in (3.10), and

$$U_{\widehat{w}_1, \widehat{w}_2}^\varepsilon(p, E) = \frac{1}{2} (U_{\widehat{w}_1, \widehat{w}_2}(p_\perp^\varepsilon, E) + U_{\widehat{w}_1, \widehat{w}_2}(p_\perp^\varepsilon, E)), \quad (3.14)$$

$$\begin{aligned} p_\pm^\varepsilon &= p_\perp + \pi z(p) \frac{y}{|y|^2} \pm \varepsilon \frac{y}{|y|^2}, \quad p_\perp = p - (p \cdot y) \frac{y}{|y|^2}, \quad p \in \mathcal{B}_{2\sqrt{E}}^d \cap Z_y^\varepsilon, \\ &\text{for the unique } z(p) \in \mathbb{Z} \text{ such that } |py - \pi z(p)| < \varepsilon. \end{aligned} \quad (3.15)$$

Then it was shown in [1, Theorem 2] that

$$\|u_E - v\|_{L^\infty(\mathbb{R}^d)} = \mathcal{O}(E^{-\alpha}) \quad E \rightarrow +\infty \quad \text{with } \alpha = \frac{\frac{1}{2}(n-d)}{n+\sigma+\frac{n-d}{2}}, \quad (3.16)$$

The geometry of vectors $p, p_\perp, y, p_\pm^\varepsilon$ is illustrated in Fig. 1 for the case when the direction of y coincides with the basis vector $e_1 = (1, 0, \dots, 0)$.

3.2 Approximate reconstruction of phased scattering data

We consider Problem 1 for $d \geq 2, L = 2$, with the unknown potential v satisfying (1.1b) and with the background potentials w_1, w_2 satisfying (1.5). Let

$$D_{\text{ext}} = D \cup \Omega_1 \cup \Omega_2, \quad (3.17)$$

where D, Ω_1, Ω_2 are the domains in (1.1b) and (1.5).

Let v_E^* be an approximation to v satisfying (2.12) for some $A > 0, \alpha \geq 0, K > 0$ and for $E^* = E^*(K, D_{\text{ext}})$, where $E^*(K, D_{\text{ext}})$ is defined according to (2.13). In addition, we suppose that

$$\|v + w_l\|_{L^\infty(\mathbb{R}^d)} \leq K, \quad \|v^*(\cdot, E) + w_l\|_{L^\infty(\mathbb{R}^d)} \leq K, \quad E \geq E^*, \quad l = 1, 2. \quad (3.18)$$

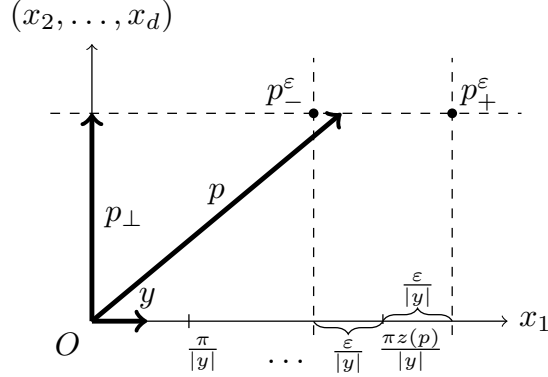


Figure 1: Vectors p , p_\perp , y and p_\pm^ε of formula (3.15)

Using the scattering amplitudes f_E^* , $f_{E,1}^*$, and $f_{E,2}^*$ of the known potentials v_E^* , $v_{E,1}^* := v_E^* + w_1$, and $v_{E,2}^* := v_E^* + w_2$, respectively, and the phaseless scattering data S of Problem 1, we construct an approximation $\tilde{f}_E^{\text{appr}}(p)$ to $(\Phi f_E)(p)$ for $|p| \leq 2\sqrt{E}$ by the function in Algorithm 1 as follows:

$$\tilde{f}_E^{\text{appr}}(p) := \text{Urec} \left(\Phi f_{E,1}^*(p) - \Phi f_E^*(p), \Phi f_{E,2}^*(p) - \Phi f_E^*(p), \Phi |f_E|^2(p), \Phi |f_{E,1}|^2(p), \Phi |f_{E,2}|^2(p) \right) \quad (3.19)$$

Note that $\tilde{f}_E^{\text{appr}}(p)$ is well defined if

$$\zeta^*(p, E) := \det \begin{pmatrix} \text{Re}(\Phi f_{E,1}^*(p) - \Phi f_E^*(p)) & \text{Im}(\Phi f_{E,1}^*(p) - \Phi f_E^*(p)) \\ \text{Re}(\Phi f_{E,2}^*(p) - \Phi f_E^*(p)) & \text{Im}(\Phi f_{E,2}^*(p) - \Phi f_E^*(p)) \end{pmatrix} \neq 0. \quad (3.20)$$

Note that condition (3.20) is satisfied for sufficiently large E at fixed $p \in \mathcal{B}_{2\sqrt{E}}^d$ if $\zeta_{\widehat{w}_1, \widehat{w}_2}(p) \neq 0$, where $\zeta_{\widehat{w}_1, \widehat{w}_2}$ is the determinant of formula (3.3). This follows from the estimate

$$|\zeta^*(p, E) - \zeta_{\widehat{w}_1, \widehat{w}_2}(p)| \leq \mu_{1, \S 3.2} E^{-\frac{1}{2}}, \quad p \in \mathcal{B}_{2\sqrt{E}}^d, \quad E \geq E^*, \quad (3.21)$$

where $\mu_{1, \S 3.2} > 0$ and $E^* = E^*(K, D_{\text{ext}})$ is defined according to (2.13), (3.17). Estimate (3.21) follows from the definition of M in Algorithm 1, the formula $M^{-1} = \frac{1}{\zeta} \begin{pmatrix} \text{Im } W_2 & -\text{Im } W_1 \\ -\text{Re } W_2 & \text{Re } W_1 \end{pmatrix}$, and from the estimates

$$\begin{aligned} |\widehat{v}(p) - \Phi f_E(p)| &\leq \mu_{2, \S 3.2} E^{-\frac{1}{2}}, \quad p \in \mathcal{B}_{2\sqrt{E}}^d, \quad E \geq E^*, \\ |\widehat{v}_l(p) - \Phi f_{E,l}(p)| &\leq \mu_{2, \S 3.2} E^{-\frac{1}{2}}, \quad p \in \mathcal{B}_{2\sqrt{E}}^d, \quad E \geq E^*, \quad l = 1, 2, \end{aligned} \quad (3.22)$$

where $\mu_{2, \S 3.2} = \mu_{2, \S 3.2}(K, D_{\text{ext}}) > 0$, $E^* = E^*(K, D_{\text{ext}})$; see, e.g., [28].

Lemma 3.1. *Let v , satisfying (1.1b), be the unknown potential of Problem 1 for $d \geq 2$, $L = 2$. Let w_1, w_2 be the same as in (1.5). Let $v^*(\cdot, E)$ be an approximation to v , satisfying (2.12) for some $A > 0$, $\alpha \geq 0$, $K > 0$ and for $E^* = E^*(K, D_{\text{ext}})$ defined according to (2.13), (3.17). Let $p \in \mathcal{B}_{2\sqrt{E}}^d$ be such that*

$$|\zeta_{\widehat{w}_1, \widehat{w}_2}(p)| \geq \delta, \quad (3.23)$$

for some fixed $\delta > 0$. Then:

$$|\zeta^*(p, E)| \geq \frac{\delta}{2}, \quad E \geq E^{**}, \quad (3.24)$$

$$\left| \Phi f_E(p) - \tilde{f}_E^{\text{appr}}(p) \right| \leq \mu_{3, \S 3.2} \delta^{-1} E^{-\alpha - \frac{1}{2}}, \quad E \geq E^{**}, \quad (3.25)$$

$$E^{**} = \max(4\mu_{1, \S 3.2}^2 \delta^{-2}, E^*), \quad (3.26)$$

where $\tilde{f}_E^{\text{appr}}$ is defined by (3.19), ζ^* is defined by (3.20), $\mu_{3, \S 3.2}$ is defined in (A.10) and $\mu_{1, \S 3.2}$ is the constant of (3.21).

Lemma 3.1 is proved in Section A.1.

The point is that the right-hand side of the estimate in (3.25) decays faster than the right-hand side of the estimate in (2.12b) as $E \rightarrow +\infty$. This is a crucial advantage of $\tilde{f}_E^{\text{appr}}$ as an approximation to the unknown phased scattering data Φf_E in comparison with Φf_E^* .

Using Lemma 3.1 we construct the iterative step for phaseless inverse scattering, see Sections 3.3 and 3.4.

3.3 Iterations for background potentials of type A

In this subsection we consider background potentials w_1, w_2 satisfying (3.5) and (3.6).

Iterative step. We consider Problem 1 for $d \geq 2, L = 2$, with the unknown potential v satisfying (1.1b) and with the background potentials w_1, w_2 satisfying (1.5), (3.5), (3.6).

Let v_E^* be an approximation to v satisfying (2.12) for some $A > 0, \alpha \geq 0, K > 0$ and $E^* = E^*(K, D_{\text{ext}})$, where $E^*(K, D_{\text{ext}})$ is defined according to (2.13), (3.17) (with $\Omega_1 = \Omega_2$).

We construct an improved approximation v_E^{**} to the unknown potential v via the scheme of Section 2.2 with Φf_E replaced by $\tilde{f}_E^{\text{appr}}$ of formula (3.19) of Section 3.2. Put

$$\begin{aligned} U_E^{**}(p) &= \tilde{f}_E^{\text{appr}}(p) - \Phi f_E^*(p) + \hat{v}_E^*(p), \\ p &\in \mathcal{B}_{2\sqrt{E}}^d, \zeta^*(p, E) \neq 0, \end{aligned} \quad (3.27)$$

where f_E^* is the scattering amplitude of v_E^* , and ζ^* is defined in (3.20).

Under assumptions (3.5), (3.6), the iterative step for phaseless inverse scattering is realized as follows.

Theorem 3.2. *Let v satisfy (1.1b) and $v \in W^{n,1}(\mathbb{R}^d)$ for some $n > d$. Let w_1, w_2 be the same as in (1.5), (3.5), (3.6). Let v_E^* be an approximation to v satisfying (2.12) for some $A > 0, \alpha \geq 0, K > 0$ and for $E^* = E^*(K, D_{\text{ext}})$, where $E^*(K, D_{\text{ext}})$ is defined according to (2.13), (3.17) (with $\Omega_1 = \Omega_2$). We suppose also that*

$$\alpha < \frac{n-d}{2(d+2\sigma)}, \quad (3.28)$$

where σ is the constant of (3.6). Let

$$v_E^{**}(x) := \begin{cases} \int_{\mathcal{B}_{r(E)}^d} e^{-ipx} U_E^{**}(p) dp, & x \in D, \\ 0, & x \notin D, \end{cases} \quad \text{where } r(E) := 2\tau E^{\frac{\beta}{n-d}} \text{ and } \beta := \frac{(\frac{1}{2} + \alpha)(n-d)}{n+2\sigma} \quad (3.29)$$

for some $\tau \in (0, 1]$. Here U_E^{**} is defined in (3.27), and \mathcal{B}_r^d is defined by (2.3).

Then there exist constants $B_1 = B_1(\tau, \|v\|_{n,1}, A, K, D_{\text{ext}}, d, \sigma, n, \mu_{1,\S 3.1})$ and $E_1 = E_1(\tau, \alpha, A, K, D, d, \sigma, n, \mu_{1,\S 3.1})$ defined in (A.20) such that

$$\|v_E^{**} - v\|_{L^\infty(D)} \leq B_1 E^{-\beta} \quad \text{for all } E \geq E_1. \quad (3.30)$$

Remark 3.3. Under assumptions of Theorem 3.2, $v_E^{**}(x)$ is well-defined for $E \geq E_1$, i.e.:

$$\begin{aligned} \zeta^*(p, E) &\neq 0 \quad \text{for } p \in \mathcal{B}_{r(E)}^d, E \geq E_1, \\ r(E) &\leq 2\sqrt{E} \quad \text{for } E \geq E_1. \end{aligned} \quad (3.31)$$

Remark 3.4. The following three conditions are equivalent:

$$\alpha < \frac{n-d}{2(d+2\sigma)}, \quad \beta < \frac{n-d}{2(d+2\sigma)}, \quad \alpha < \beta, \quad (3.32)$$

where β is defined in (3.29), $n > d, \alpha > 0$, and $\sigma > d$.

Theorem 3.2 is proved in Section A.2.

Theorem 3.2 of the present work can be considered as an extension of Theorem 1 of [1] to the case when $v^* \neq 0$. However, Theorem 3.2 of the present work for $v^* = 0$ does not coincide with Theorem 1 of [1].

Iterations Let v, w_1, w_2 satisfy the assumptions of Theorem 3.2. Let $u_E^{(1)} = v_E^{**}$ for $v^* = 0$. Note that $u_E^{(1)}$ is similar but does not coincide with the approximate reconstruction of Theorem 1 of [1]; see formulas (3.12), (3.11) of the present work. In particular, we have that

$$\|u_E^{(1)} - v\|_{L^\infty(D)} = \mathcal{O}(E^{-\alpha_1}), \quad E \rightarrow +\infty \text{ with } \alpha_1 := \frac{1}{2} \frac{n-d}{n+2\sigma}. \quad (3.33)$$

Then, applying the iterative step described above in this subsection we construct nonlinear approximate reconstructions $u_E^{(j)}, j \geq 2$, such that

$$\|u_E^{(j)} - v\|_{L^\infty(D)} = \mathcal{O}(E^{-\alpha_j}), \quad E \rightarrow +\infty \text{ with } \alpha_j := \frac{1}{2} \frac{n-d}{d+2\sigma} \left(1 - \left(\frac{n-d}{n+2\sigma}\right)^j\right). \quad (3.34)$$

The approximations $u_E^{(j)}$ of (3.34) for phaseless inverse scattering under assumptions (3.5), (3.6) are analogs of approximations $u_E^{(j)}$ of (2.9) for phased inverse scattering. In a similar way with (2.10),

$$\begin{aligned} \alpha_j &\rightarrow \alpha_\infty = \frac{1}{2} \frac{n-d}{d+2\sigma} && \text{as } j \rightarrow +\infty, \\ \alpha_j &\rightarrow \frac{j}{2} && \text{as } n \rightarrow +\infty, \\ \alpha_\infty &\rightarrow +\infty && \text{as } n \rightarrow +\infty, \end{aligned} \quad (3.35)$$

so that the convergence in (3.34) as $E \rightarrow +\infty$ is much more optimal than the convergence in (3.12), at least, for large j, n .

3.4 Iterations for background potentials of type B

In this subsection we consider Problem 1 for $d \geq 2$ with shifted background potentials w_1, w_2 described by (3.6), and (3.8) and unknown potential v satisfying (1.1b).

Iterative step. We consider the set Z_y^ε of formula (3.10). Put

$$\begin{aligned} p^\varepsilon(p_\perp, z, t) &= p_\perp + \pi z \frac{y}{|y|^2} + t\varepsilon \frac{y}{|y|^2}, \\ p_\perp &\in \mathbb{R}^d, \quad p_\perp \cdot y = 0, \quad z \in \mathbb{Z}, \quad t \in \mathbb{R}. \end{aligned} \quad (3.36)$$

Note that

$$\begin{aligned} &\text{for any } p \in Z_y^\varepsilon \text{ there exists the unique triple } (p_\perp, z, t) \text{ such that} \\ &p^\varepsilon(p_\perp, z, t) = p, \quad p_\perp \in \mathbb{R}^d, \quad p_\perp \cdot y = 0, \quad z \in \mathbb{Z}, \quad t \in (-1, 1). \end{aligned} \quad (3.37)$$

In addition to U^{**} of (3.27), we also define

$$U_{N,\varepsilon}^{**}(p^\varepsilon(p_\perp, z, t), E) = \sum_{-N \leq j \leq N, j \neq 0} U^{**}(p^\varepsilon(p_\perp, z, j), E) L_j(t), \quad (3.38)$$

under the assumptions that

$$\varepsilon < \frac{\pi}{N+1}, \quad |p^\varepsilon(p_\perp, z, t)| \leq 2\sqrt{E} - \frac{\pi}{|y|}, \quad t \in (-1, 1), \quad \varepsilon > 0, \quad N \geq 1, \quad (3.39)$$

where

$$L_j(t) = \frac{(-1)^{N-j} j(t+j)}{(N-j)!(N+j)!} \prod_{1 \leq i \leq N, i \neq j} (t^2 - i^2), \quad j = \pm 1, \dots, \pm N. \quad (3.40)$$

Note that for fixed $p_\perp \in \mathbb{R}^d, p_\perp \cdot y = 0$, and for fixed $z \in \mathbb{Z}$, function $U_{N,\varepsilon}^{**}(p^\varepsilon(p_\perp, z, t), E)$ is the Lagrange interpolating polynomial of degree $2N-1$ in $t \in \mathbb{R}$ for $U^{**}(p^\varepsilon(p_\perp, z, t), E)$ with the nodes at $t = \pm 1, \dots, \pm N$. In addition, $L_j(t)$ is the j -th elementary Lagrange interpolating polynomial of degree $2N-1$:

$$L_j(t) = \begin{cases} 1, & t = j, \\ 0, & t = \pm 1, \dots, \pm N, \quad t \neq j. \end{cases} \quad (3.41)$$

Note also that if assumptions (3.39) are valid for some $p_\perp \in \mathbb{R}^d$, $p_\perp \cdot y = 0$, $z \in \mathbb{Z}$, $t \in (-1, 1)$, then

$$p^\varepsilon(p_\perp, z, s) \in \mathcal{B}_{2\sqrt{E}}^d \setminus Z_y^\varepsilon \quad \text{for all } s \in [-N, -1] \cup [1, N]. \quad (3.42)$$

Under assumptions (3.6), (3.8), the iterative step is realized as follows.

Theorem 3.5. *Let v satisfy (1.1b) and $v \in W^{n,1}(\mathbb{R}^d)$ for some $n > d$. Let w_1, w_2 be the same as in (1.5), (3.6), (3.8). Let v_E^* be an approximation to v satisfying (2.12a), (2.12) for some $A > 0$, $\alpha \geq 0$, $K > 0$ and for $E^* = E^*(K, D_{ext})$, where $E^*(K, D_{ext})$ is defined according to (2.13), (3.17) (with $\Omega_1 = \Omega_2$). We suppose also that*

$$\alpha < \frac{n-d}{2(d+2\sigma+\frac{n-d}{2N+1})} \quad \text{for some } N \geq 1, \quad (3.43)$$

where σ is the constant of (3.6). Let

$$v_E^{**}(x) := \begin{cases} \int_{\mathcal{B}_{r(E)}^d \setminus Z_y^{\varepsilon(E)}} e^{-ipx} U_E^{**}(p) dp, & \int_{\mathcal{B}_{r(E)}^d \cap Z_y^{\varepsilon(E)}} e^{-ipx} U_{N,\varepsilon(E)}^{**}(p, E) dp & x \in D \\ 0, & & x \notin D \end{cases} \quad (3.44)$$

with $r(E) = 2\tau E^{\frac{\beta}{n-d}}$, $\varepsilon(E) = E^{-\frac{\beta}{2N+1}}$, $\beta = \frac{(\frac{1}{2}+\alpha)(n-d)}{n+2\sigma+\frac{n-d}{2N+1}}$, for some $\tau \in (0, 1]$,

where U_E^{**} is defined by formulas (3.27); $U_{N,\varepsilon}^{**}(p, E)$ is defined by (3.38); \mathcal{B}_r^d , Z_y^ε are defined by (2.3), (3.10).

Then the following estimate holds:

$$\|v_E^{**} - v\|_{L^\infty(D)} \leq B_2 E^{-\beta}, \quad E \geq E_2, \quad (3.45)$$

where $B_2 = B_2(\tau, y, N, \|v\|_{n,1}, A, K, D_{ext}, d, \sigma, n, \mu_{1,\S 3.1})$ and $E_2 = E_2(\tau, y, \alpha, N, A, K, D, d, \sigma, n, \mu_{1,\S 3.1})$ are defined in (A.49).

Theorem 3.5 is proved in Section A.3.

Remark 3.6. *Under assumptions of Theorem 3.5, $v_{E,1}^{**}(x)$ and $v_{E,2}^{**}(x)$ are well-defined for $E \geq E_2$, i.e.:*

$$\begin{aligned} \zeta^*(p, E) &\neq 0 \quad \text{for } p \in \mathcal{B}_{r(E)}^d \setminus Z_y^{\varepsilon(E)}, \quad E \geq E_2, \\ r(E) &\leq 2\sqrt{E} \quad \text{for } E \geq E_2, \end{aligned} \quad (3.46)$$

where ζ^* is defined by (3.20), and also

$$\varepsilon(E) < \frac{\pi}{N+1}, \quad |p| \leq 2\sqrt{E} - \frac{\pi}{|y|} \quad \text{for } p \in \mathcal{B}_{r(E)}^d, \quad E \geq E_2. \quad (3.47)$$

Remark 3.7. *The following three conditions are equivalent:*

$$\alpha < \frac{n-d}{2(d+2\sigma+\frac{n-d}{4N+1})}, \quad \beta < \frac{n-d}{2(d+2\sigma+\frac{n-d}{4N+1})}, \quad \alpha < \beta, \quad (3.48)$$

where β is defined in (3.44), $n > d$, $\alpha > 0$, and $\sigma > d$. In addition, each of conditions (3.48) is equivalent to the following pair of conditions:

$$\alpha < \frac{n-d}{2(d+2\sigma)}, \quad N > \frac{1}{2} \left(\alpha^{-1} - \left(\frac{n-d}{2(d+2\sigma)} \right)^{-1} \right)^{-1} - \frac{1}{4}. \quad (3.49)$$

Iterations. Let v, w_1, w_2 satisfy the assumptions of Theorem 3.5. Let $u_E^{(1)} = v_E^{**}$ for $v^* = 0$. Note that $u_E^{(1)}$ is similar, but does not coincide with the approximate reconstruction of Theorem 2 of [1]; see formulas (3.16), (3.13) of the present article. In particular, we have that

$$\|u_E^{(1)} - v\|_{L^\infty(D)} + \mathcal{O}(E^{-\alpha_1}), \quad E \rightarrow +\infty \quad \text{with } \alpha_1 = \frac{1}{2} \frac{n-d}{n+2\sigma+\frac{n-d}{2N+1}}. \quad (3.50)$$

Then, applying the iterative step described above in this subsection we construct nonlinear approximate reconstructions $u_E^{(j)}$, $j \geq 2$, such that

$$\|u_E^j - v\|_{L^\infty(D)} = \mathcal{O}(E^{-\alpha_j}) \quad E \rightarrow +\infty \quad \text{with } \alpha_j = \frac{1}{2} \frac{n-d}{d+2\sigma+\frac{n-d}{2N+1}} \left(1 - \left(\frac{n-d}{n+2\sigma+\frac{n-d}{2N+1}}\right)^j\right). \quad (3.51)$$

These approximations $u^{(j)}$ for phaseless inverse scattering under assumptions (3.6), (3.8) are analogs of approximations $u^{(j)}$ of (2.9) for phased inverse scattering. In a similar way with (2.10) and (3.35),

$$\begin{aligned} \alpha_j &\rightarrow \alpha_\infty = \frac{1}{2} \frac{n-d}{d+2\sigma+\frac{n-d}{2N+1}} \quad \text{as } j \rightarrow +\infty, \\ \alpha_j &\rightarrow \frac{j}{2} \quad \text{as } n \rightarrow +\infty, N \rightarrow +\infty, \\ \alpha_\infty &\rightarrow +\infty \quad \text{as } n \rightarrow +\infty, \end{aligned} \quad (3.52)$$

so that the convergence in (3.51) as $E \rightarrow +\infty$ is much faster than the convergence in (3.16), at least, for large j , n , N .

4 Numerical experiments

4.1 Implementation of the Fourier transform and its inverse

The iterative algorithm presented in sections 3.3, 3.4 is implemented in `Matlab` in the two-dimensional case. In our implementation we represent potentials v and w_l by discrete functions \underline{v} , \underline{w}_l defined on the space-variable grid

$$\begin{aligned} \Gamma^s &:= \left\{ \frac{2}{N}(n_1, n_2) : n_1, n_2 \in \mathbb{Z}_N \right\} \text{ for } N \in 2\mathbb{N}, N \geq \frac{2\sqrt{E}}{\pi} \\ \text{where } \mathbb{Z}_N &:= \left\{ -\frac{N}{2}, -\frac{N}{2} + 1, \dots, \frac{N}{2} - 1 \right\}. \end{aligned} \quad (4.1)$$

In turn, the input data $|f(k, l)|^2$, $|f_l(k, l)|^2$ are measured on a grid

$$\mathcal{M}_E^m = \{(k_m, l_m) : m = 1..M\} \subset \mathcal{M}_E,$$

whose precise form depends on the experimental setup. This leads to the following grid in Fourier space:

$$\Gamma^m := \{k_m - l_m : m = 1..M\}$$

Minimal data. To approximate the inverse Fourier transform of a function, which is supported on $\mathcal{B}_{2\sqrt{E}}^2$ and sampled on the grid Γ^m , by the Fast Fourier transform (FFT), Γ^m has to be rectangular. If Γ^s is given by (4.1), a minimal choice of Γ^m is

$$\Gamma_{\min}^m := \mathcal{B}_{2\sqrt{E}}^2 \cap \pi\mathbb{Z}^2. \quad (4.2)$$

A corresponding measurement grid $\mathcal{M}_{E, \min}^m$ can be defined as in (2.4) replacing $\mathcal{B}_{2\sqrt{E}}^2$ by Γ_{\min}^m . Extending a function given on Γ^m to the exterior grid

$$\Gamma^e := \{\pi(n_1, n_2) : n_1, n_2 \in \mathbb{Z}_N, \pi^2(n_1^2 + n_2^2) > 4E\} \quad (4.3)$$

by 0, we can compute an approximation to the inverse Fourier transform on Γ^s by FFT.

Discrete Ewald circles. The above choice Γ_{\min}^m of the set of measurement points is inconvenient both from an experimental and from a computational point of view since each point in Γ_{\min}^m corresponds to a different incident wave. If a scattering experiment is performed for some incident wave or if the solution to the scattering problem is computed numerically, the resulting far field pattern can be evaluated at other points without essential additional costs.

Therefore, we now consider input data for M_1 uniformly distributed incident wave vectors k where each far field pattern is evaluated at M_2 uniformly distributed scattered wave vectors l :

$$\begin{aligned} k(s) &:= \sqrt{E} \left(\cos(2\pi \frac{s}{M_1}), \sin(2\pi \frac{s}{M_1}) \right), \\ l(s, t) &:= \sqrt{E} \left(\cos(\frac{2\pi s}{M_1} + \frac{2\pi t}{M_2}), \sin(\frac{2\pi s}{M_1} + \frac{2\pi t}{M_2}) \right), \end{aligned} \quad s \in \mathbb{Z}_{M_1}, t \in \mathbb{Z}_{M_2}, \quad (4.4)$$

resulting in

$$\mathcal{M}_{E, M_1, M_2}^m := \{ (k(s), l(s, t)) \mid s \in \mathbb{Z}_{M_1}, t \in \mathbb{Z}_{M_2} \}, \quad M = M_1 M_2, \quad (4.5)$$

$$\Gamma_{M_1, M_2}^m := \{ k - l : (k, l) \in \mathcal{M}_{E, M_1, M_2}^m \}. \quad (4.6)$$

This is illustrated in Fig. 2: The points of $\Gamma^m = \Gamma_{M_1, M_2}^m$ corresponding to a given incident wave vector k are located on the red circle passing through the origin O and centered at point O' such that $\overrightarrow{OO'} = k$. These points of Γ^m corresponding to a fixed k are also called (discrete) Ewald circle in the physical literature.

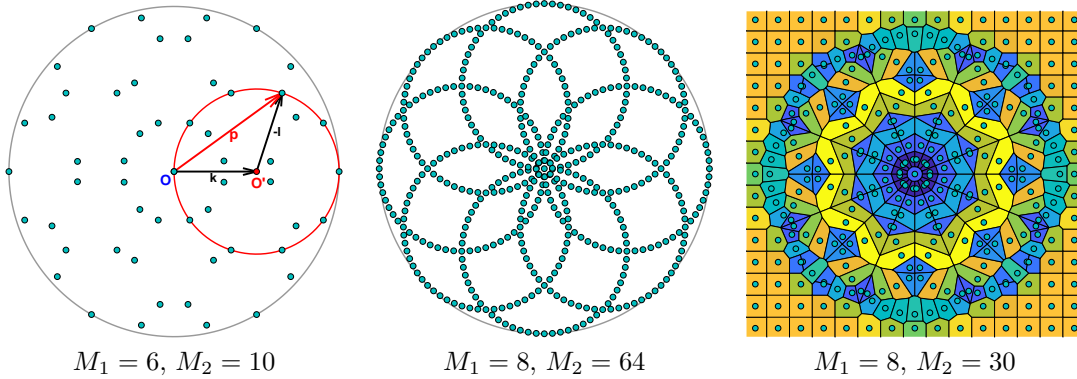


Figure 2: Illustration of sets of transformed measurement points Γ_{M_1, M_2}^m on Discrete Ewald circles for different values of the numbers M_1 of incident waves and far field points M_2 . The right panel shows the Voronoi diagram corresponding to the grid $\Gamma^e \cup \Gamma_{M_1, M_2}^m$. The color is related to the area of a cell.

Given a discrete function $\underline{v}: \Gamma^s \rightarrow \mathbb{C}$ representing a function $v: \mathbb{R}^2 \rightarrow \mathbb{C}$, the Fourier transform of v can be approximately represented by a discrete function $\widehat{\underline{v}}: \Gamma^m \cup \Gamma^e \rightarrow \mathbb{C}$ such that $\widehat{\underline{v}} = A\underline{v}$, where

$$A := \left[(N\pi)^{-2} \exp(ix \cdot p) \right]_{p \in \Gamma^m \cup \Gamma^e, x \in \Gamma^s}.$$

Here it is necessary to include the points in Γ^e to obtain small condition numbers of A since the inverse Fourier transform is computed by numerically inverting A . Matrix-vector products with A and A^* can be computed efficiently without the need to set up and store the matrix A using the Nonequispaced Fast Fourier Transform (NFFT). In our work we use the NFFT implementation of [19]. The definitions of the grids Γ^s , Γ^m , Γ^e and of the Fourier transform matrix A are summarized in Algorithm 2.

Approximation of the inverse Fourier transform. A first idea may be to approximate the continuous inverse Fourier transform by the Moore-Penrose inverse of A . If A is injective, this corresponds to the solution of a least-squares problem

$$A^\dagger \underline{U} = \operatorname{argmin}_{\underline{w}} \|A\underline{w} - \underline{U}\|_2^2$$

which can be achieved by the conjugate gradient (CG) method applied to the normal equation $(A^*A)\underline{w} = A^*\underline{U}$. The ideal situation would be that A is isometric, i.e. $\|A\underline{w}\|_2 = \|\underline{w}\|_2$ for all $\underline{w}: \Gamma^s \rightarrow \mathbb{C}$. In this case $A^\dagger = A^*$, and the CG method would yield the exact solution in the

Algorithm 2 function $[\Gamma^m, \Gamma^e, A, \Phi] = \text{fourier_setup}(\Gamma^s, \mathcal{M}_E^m)$

data: spatial grid: $\Gamma^s := \{\frac{2}{N}(n_1, n_2) : n_1, n_2 \in \mathbb{Z}, -\frac{N}{2} \leq n_1, n_2 < \frac{N}{2}\}$ with $N \in 2\mathbb{N}$, $N \geq \frac{2\sqrt{E}}{\pi}$

measurement points: $\mathcal{M}_E^m = \{(k_m, l_m) : m = 1..M\} \subset \mathcal{M}_E$

results: Fourier space grids inside and outside $\mathcal{B}_{2\sqrt{E}}^2$: Γ^m, Γ^e

matrix representing Fourier transform: A

pushforward matrix from the measurement grid \mathcal{M}_E^m to the Fourier space grid Γ^m : Φ

$\Gamma^m := \{k_m - l_m : m = 1..M\};$ \triangleright grid inside $\mathcal{B}_{2\sqrt{E}}^2$

$\Gamma^e := \{\pi(n_1, n_2) : n_1, n_2 \in \mathbb{Z}, -\frac{N}{2} \leq n_1, n_2 < \frac{N}{2}, \pi^2(n_1^2 + n_2^2) > 4E\};$ \triangleright grid outside $\mathcal{B}_{2\sqrt{E}}^2$

$A := [(\pi N)^{-2} \exp(ix \cdot p)]_{p \in \Gamma^m \cup \Gamma^e, x \in \Gamma^s};$ \triangleright avoid computation of A and use NFFT instead

$(\Phi \underline{f})_p := \frac{1}{\#(M_p)} \sum_{m \in M_p} \underline{f}_m$ where $M_p := \{m : k_m - l_m = p\}$

first step. However, in our situation A is typically far from being isometric, so that A^*A is far from the identity matrix, and the CG method requires a big number of iterations. The reason is that even though the continuous Fourier transform is isometric, the Euclidean norm $\|\underline{U}\|_2$ of the sampled version $\underline{U} : \Gamma^m \cap \Gamma^e \rightarrow \mathbb{C}$ of a function $U : [-\frac{N\pi}{2}, \frac{N\pi}{2}]^2 \rightarrow \mathbb{C}$ can be a bad approximation for $\|U\|_{L^2}$.

To overcome this difficulty, we design a weight matrix D such that $\|D^{1/2}\underline{U}\|_2 \approx \|U\|_{L^2}$. Then we approximate the inverse Fourier transform by the Moore-Penrose inverse of A with respect to this weighted norm $\|D^{1/2} \cdot\|_2$, or in matrix notation

$$(D^{1/2}A)^\dagger D^{1/2}\underline{U} = \text{argmin}_{\underline{w}} \|D^{1/2}A\underline{w} - D^{1/2}\underline{U}\|_2^2.$$

Recall that by the first-order optimality conditions, which are necessary and sufficient for convex functionals, this minimization problem is equivalent to solving the normal equation $A^*DA\underline{w} = A^*D\underline{U}$.

To construct a matrix D such that $\|D^{1/2}\underline{U}\|_2^2 \approx \int |U(p)|^2 dp$, we use a Voronoi partition of the square $[-\frac{\pi N}{2}, \frac{\pi N}{2}]^2$ into cells $C(p)$ centered at points $p \in \Gamma^m \cup \Gamma^e$. In `Matlab` this subdivision is computed by the built-in function `voronoi`, see Fig. 2. To approximate the integral by a Riemann sum we evaluate the area $|C(p)|$ of each cell $C(p)$, $p \in \Gamma^m \cup \Gamma^e$ and choose D as the diagonal matrix $D := \text{diag}(|C(p)|)_{p \in \Gamma^m \cup \Gamma^e}$. The use of this matrix D drastically decreases the number of CG steps and allows the approximate evaluation of the inverse Fourier transform with just a few CG steps. The reason is that A^*DA is much closer to the identity matrix as A^*A .

Remark 4.1. *If the function \underline{U} is defined only on some subgrid $G \subset \Gamma^m \cup \Gamma^e$, two minor modifications are necessary: (i) The Fourier matrix A must be restricted to the grid G yielding matrix $\hat{A} = [A_{pq}]_{p \in \Gamma, q \in G}$; (ii) The matrix of Voronoi weights D must be computed for the grid G .*

4.2 Implementation of the inversion method

Phaseless Born approximation. Recall that in our implementation the potentials w_l are represented by discrete functions $\underline{w}_l : \Gamma^s \rightarrow \mathbb{C}$, and the measured phaseless farfield data $|f|^2, |f_l|^2$ are represented by the discrete functions \underline{F} and $\underline{F}_l : \mathcal{M}_E^m \rightarrow \mathbb{R}$. Also note that in addition to the background potentials and phaseless farfield data, a cutoff radius $r_1 > 0$ and a threshold $\delta > 0$ are specified as input data for the algorithm. The cutoff radius $0 < r_1 \leq 2\sqrt{E}$ is analogous to the radius $r(E)$ of formulas (3.11), (3.13), whereas the threshold δ is analogous to threshold $\varepsilon(E)$ of formula (3.13).

The implementation of the phaseless Born approximation is shown in Algorithm 3. The algorithm is formulated for an arbitrary number $L \geq 2$ of reference potentials, but reduces to the algorithm in the theoretical part of this paper if $L = 2$. The principal part is the computation of the reduced grid $\tilde{\Gamma}^m \subset \Gamma^m$, which consists of points $p \in \Gamma^m$ meeting the threshold and the cutoff constraints, and of the function $\underline{U} : \tilde{\Gamma}^m \cup \Gamma^e \rightarrow \mathbb{C}$, which is the discrete version of the function

$U_{\widehat{w}_1, \widehat{w}_2}$ of Subsection 3.1. This computation starts by initializing $\tilde{\Gamma}^m$ by the empty grid and \underline{U} by the zero function and proceeds as follows:

1. For each point $p \in \Gamma^m$ and each pair $w_{\tilde{l}}, w_l$ of reference potentials, compute the determinant $\zeta_{\underline{p}}^{\tilde{l}, l}$ corresponding to $\zeta_{\widehat{w}_1, \widehat{w}_2}(p)$ of formula (3.3). Since the approximate Fourier transform \underline{U}_p of \underline{v} can be computed from any pair (\tilde{l}, l) for which $\zeta_{\underline{p}}^{\tilde{l}, l} \neq 0$ and since the computation is the more stable the larger $|\zeta_{\underline{p}}^{\tilde{l}, l}|$, we choose the pair $(\tilde{l}(p), l(p))$, for which $|\zeta_{\underline{p}}^{\tilde{l}, l}|$ is largest.
2. If $|\zeta_{\underline{p}}^{\tilde{l}(p), l(p)}| > \delta$ (threshold constraint) include p in $\tilde{\Gamma}^m$. In addition, if $|p| < r_1$ (cutoff constraint) compute \underline{U}_p using Algorithm 1 with appropriate parameters. Rather than implementing an explicit interpolation scheme at points where $\zeta_{\underline{p}}^{\tilde{l}(p), l(p)}$ vanishes or is too small as done in (3.14) for our theoretical analysis, we use a trigonometric interpolation of the discrete Fourier transform induced by fitting to the remaining points of Γ^m . This procedure is easier to implement and allows the numerical treatment of arbitrary background potentials.

The last step is to compute the function $\underline{v}_E^*: \Gamma^s \rightarrow \mathbb{C}$, which is the discrete version of the phaseless Born approximation u_E of Subsection 3.1, as the inverse Fourier transform of the function represented by \underline{U} . This step is explained in Subsection 4.1.

Algorithm 3 function $[v_E^*, \tilde{\Gamma}^m, \tilde{A}, D] = \text{phaseless_born_inv}(F_0, F_1, w_1, \dots, F_L, w_L, \Gamma^s, \mathcal{M}_E^m, r_1, \delta)$

data: measured data $(F_0)_m \approx |f(k_m, l_m)|^2$, $(F_l)_m \approx |f_l(k_m, l_m)|^2$ for $m = 1..M$, $l = 1..L$

(discrete) background potentials $\underline{w}_1, \dots, \underline{w}_L: \Gamma^s \rightarrow \mathbb{C}$

Γ^s , \mathcal{M}_E^m as in `fourier_setup`

cutoff radius $r_1 > 0$

threshold $\delta > 0$

results: potential reconstruction: \underline{v}_E^*

reduced Fourier space grid and Fourier transform matrix: $\tilde{\Gamma}^m, \tilde{A}$

Voronoi diagonal weight matrix: D

$[\Gamma^m, \Gamma^e, A, \Phi] = \text{fourier_setup}(\Gamma^s, \mathcal{M}_E^m);$

▷ see Algorithm 2

$\widehat{w}_l := A \underline{w}_l$ for $l = 1, \dots, L;$

▷ use NFFT

$\mathcal{P} := \{(\tilde{l}, l) \in \{1, \dots, L\}^2: \tilde{l} < l\};$

$\tilde{\Gamma}^m := [];$ $\underline{U}_p := 0$ for $p \in \Gamma^m \cup \Gamma^e;$

for $p \in \Gamma^m$ **do**

for $(\tilde{l}, l) \in \mathcal{P}$ **do**

$\zeta_{\underline{p}}^{\tilde{l}, l} = \text{Re } \widehat{w}_{\tilde{l}, p} \text{ Im } \widehat{w}_{l, p} - \text{Im } \widehat{w}_{\tilde{l}, p} \text{ Re } \widehat{w}_{l, p};$

end for

Choose $(\tilde{l}(p), l(p)) \in \text{argmax}_{(\tilde{l}, l) \in \mathcal{P}} |\zeta_{\underline{p}}^{\tilde{l}, l}|;$

if $|\zeta_{\underline{p}}^{\tilde{l}(p), l(p)}| > \delta$ **then**

$\tilde{\Gamma}^m := \tilde{\Gamma}^m \cup \{p\};$

if $|p| < r_1$ **then**

$\underline{U}_p := \text{Urec}(\widehat{w}_{\tilde{l}(p), p}, \widehat{w}_{l(p), p}, (\Phi F_0)_p, (\Phi F_{\tilde{l}(p)})_p, (\Phi F_{l(p)})_p);$

▷ see Algorithm 1

end if

end if

end for

$\tilde{A} := [A_{px}]_{p \in \tilde{\Gamma}^m \cup \Gamma^e, x \in \Gamma^s};$

$D := \text{voronoi_weights}(\tilde{\Gamma}^m \cup \Gamma^e);$

$\underline{v}_E^* := (D^{1/2} \tilde{A})^\dagger D^{1/2} [\underline{U}_p]_{p \in \tilde{\Gamma}^m \cup \Gamma^e};$

▷ may be computed by CG and NFFT

Iterative algorithm. In addition to the input parameters of the phaseless Born approximation, the iterative algorithm requires cutoff radii $0 < r_1 \leq \dots \leq r_J \leq 2\sqrt{E}$ to be specified. The implementation of the iterative method is shown in Algorithm 4.

The first step is the computation of the phaseless Born approximation $\underline{v}_E^* : \Gamma^s \rightarrow \mathbb{C}$, as well as of the grids $\Gamma^m, \Gamma^e, \tilde{\Gamma}^m$, Fourier matrices A, \tilde{A} and Voronoi's matrix of weights D , as explained above. The main part of the algorithm is the iteration procedure producing improved approximations \underline{v}_E^* .

The iterative step starts by evaluating the scattering amplitudes f_E^* and $f_{E,l}^*$, $l = 1, \dots, L$ of the potentials represented by discrete functions $\underline{v}_E^*, \underline{v}_E^* + \underline{w}_l$ at the points of the grid \mathcal{M}_E^m yielding discrete functions $\underline{f}_E^*, \underline{f}_{E,l}^* : \mathcal{M}_E^m \rightarrow \mathbb{C}$. In principle, any black-box solver can be used to evaluate the scattering amplitudes. In our work we use the solver described in [31, 15].

The iterative step proceeds by computing the discrete function $\tilde{f}_E^{\text{appr}} : \tilde{\Gamma}^m \cup \Gamma^e \rightarrow \mathbb{C}$, which is the discrete analog of function $\tilde{f}_E^{\text{appr}}$ of (3.19), as well as the function $\underline{U}^{**} : \tilde{\Gamma}^m \cup \Gamma^e \rightarrow \mathbb{C}$, which is analogous to function U_E^{**} of (3.27). This computation starts by initializing $\tilde{f}_E^{\text{appr}}$ and \underline{U}^{**} by the zero functions and continues as follows:

1. For each point $p \in \tilde{\Gamma}^m$ such that $|p| < r_j$, where $j \geq 2$ is the current iteration number⁴, compute $(\tilde{f}_E^{\text{appr}})_p$ using Algorithm 1 with appropriate parameters. If $L \geq 3$ reference potentials are available, we again choose the most stable pair at each point p .
2. Evaluate \underline{U}_p^{**} according to formula (3.27).

The iteration ends by computing \underline{v}_E^* , as the inverse Fourier transform of the function represented by \underline{U}^{**} . The computation is explained in Subsection 4.1.

Algorithm 4 function $\underline{v}_E^* = \text{phaseless_iterative_inv}(\underline{E}_0, \underline{E}_1, \underline{w}_1, \dots, \underline{E}_L, \Gamma^s, \mathcal{M}_E^m, \underline{w}_L, r_1 \dots r_J, \delta)$

data: measured data $(\underline{E}_0)_m \approx |f(k_m, l_m)|^2$, $(\underline{E}_l)_m \approx |f_l(k_m, l_m)|^2$ for $m = 1..M$, $l = 1..L$

(discrete) background potentials $\underline{w}_1, \dots, \underline{w}_L : \Gamma^s \rightarrow \mathbb{C}$

$\Gamma^s, \mathcal{M}_E^m$ as in `fourier_setup`

cutoff radii $0 < r_1 \leq r_2 \leq \dots \leq r_J \leq 2\sqrt{E}$

threshold $\delta > 0$

result: potential reconstruction \underline{v}_E^*

$[\Gamma^m, \Gamma^e, A, \Phi] := \text{fourier_setup}(\Gamma^s, \mathcal{M}_E^m);$ ▷ see Algorithm 2

$[\underline{v}_E^*, \tilde{\Gamma}^m, \tilde{A}, D] := \text{phaseless_born_inv}(\underline{E}, \underline{E}_1, \underline{w}_1, \dots, \underline{w}_L, \underline{E}_L, \Gamma^s, \mathcal{M}_E^m, r_1, \delta);$ ▷ see Alg. 3

$\mathcal{P} := \{(\tilde{l}, l) \in \{1, \dots, L\}^2 : \tilde{l} < l\};$

for $j = 2, \dots, J$ **do**

$\underline{f}_E^* := \text{scattering_amplitude}(\underline{v}_E^*);$ ▷ Solve phased forward problem

$\underline{f}_{E,l}^* := \text{scattering_amplitude}(\underline{v}_E^* + \underline{w}_l)$ for $l = 1..L;$

$\tilde{f}_E^{\text{appr}} := 0; \quad \underline{U}_p^{**} := 0$ for $p \in \tilde{\Gamma}^m \cup \Gamma^e;$ ▷ grid functions on $\tilde{\Gamma}^m \cup \Gamma^e$

for $p \in \tilde{\Gamma}^m$ such that $|p| < r_j$ **do**

Choose $(\tilde{l}(p), l(p)) \in \arg\max_{(\tilde{l}, l) \in \mathcal{P}} \text{Re} \hat{w}_{\tilde{l}, p} \text{Im} \hat{w}_{l, p} - \text{Im} \hat{w}_{\tilde{l}, p} \text{Re} \hat{w}_{l, p};$

$(\tilde{f}_E^{\text{appr}})_p := \text{Urec} \left((\Phi \underline{f}_{E, \tilde{l}(p)}^* - \Phi \underline{f}_E^*)_p, (\Phi \underline{f}_{E, l(p)}^* - \Phi \underline{f}_E^*)_p, (\Phi \underline{E}_0)_p, (\Phi \underline{E}_{\tilde{l}(p)})_p, (\Phi \underline{E}_{l(p)})_p \right);$

$\underline{U}_p^{**} := (A \underline{v}_E^*)_p + (\tilde{f}_E^{\text{appr}})_p - (\Phi \underline{f}_E^*)_p;$

end for

$\underline{v}_E^* := (D^{1/2} \tilde{A})^\dagger D^{1/2} \underline{U}^{**};$ ▷ may be computed by CG and NFFT

end for

⁴by convention, $j = 1$ corresponds to phaseless Born approximation

4.3 Numerical results

Reconstruction errors. We consider the reconstruction of the potential v shown in Fig. 3 (a)⁵ using three background potentials w_1, w_2, w_3 shown at Fig. 3 (b), (c), (d). The differential scattering cross-section of the potential v for the incident direction $k = \sqrt{E}(-1, 0)$ at $E = 10^2$ and $E = 20^2$ is shown at Fig. 4. One can see that for bigger energy the differential scattering cross-section is more concentrated near $l \approx k$.

In the experiments 32 equidistant incident directions and 256 equidistant measurement directions (for each k) were used. Moreover we choose $N \approx c\sqrt{E}$ with $c = 5$ so that the space grid discretization step is $2/N \approx 0.4/\sqrt{E}$. For simplicity, we choose uniformly increasing cutoff radii $r_j = \sqrt{E}(1 + \frac{j}{J+1})$.

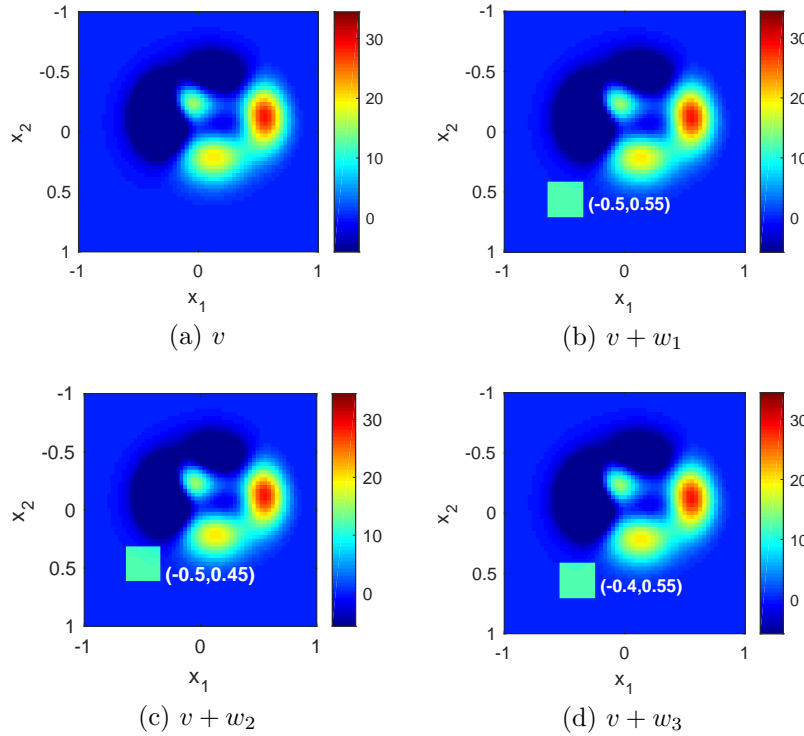


Figure 3: Unknown potential and background potentials

In quantum mechanical and optical applications the dominant source of noise is often caused by the limited number N_p of measured particles, leading to Poisson distributed data. More precisely, recall that the quantity $|f(k, l)|^2$ is proportional to the probability density of scattering of a particle with initial momentum k into direction $l/|l| \neq k/|k|$. Let $K := \#\{k_1, \dots, k_m\}$ denote the number of incident waves. We assume that for each background potential and each incident wave the exposure time $t_l(k_m)$ is chosen such that the same expected number of particles $N_p/K(L+1)$ is recorded. Thus, our simulated noisy data $\underline{E} := [E_0, E_1, \dots, E_L]$, were generated from exact data $\underline{E}^\dagger := [E_0^\dagger, E_1^\dagger, \dots, E_L^\dagger]$ with $(E_0^\dagger)_m := |f(k_m, l_m)|^2$ and $(E_l^\dagger)_m := |f_l(k_m, l_m)|^2$, $l = 1, \dots, L$ by

$$(\underline{E}_l)_m \sim \frac{1}{t_l(k_m)} \text{Pois} \left(t_l(k_m) (E_l^\dagger)_m \right) \quad \text{with } t_l(k_m) := \frac{N_p}{K(L+1)\sigma_l(k_m)}, \quad \sigma_l(k_m) := \sum_{n: k_n=k_m} (E_l^\dagger)_n$$

(see [16] for more details). Here $\text{Pois}(x)$ stands for a Poisson random variable with mean x . Recall that $\mathbf{E}(\underline{E}_l)_m = (E_l^\dagger)_m$ and that the pointwise noiselevel is $\sqrt{\text{Var}(\underline{E}_l)_m} = t_l(k_m)^{-1/2} \sqrt{(E_l^\dagger)_m}$. For

⁵this potential is given by the `Matlab`'s function `peaks`

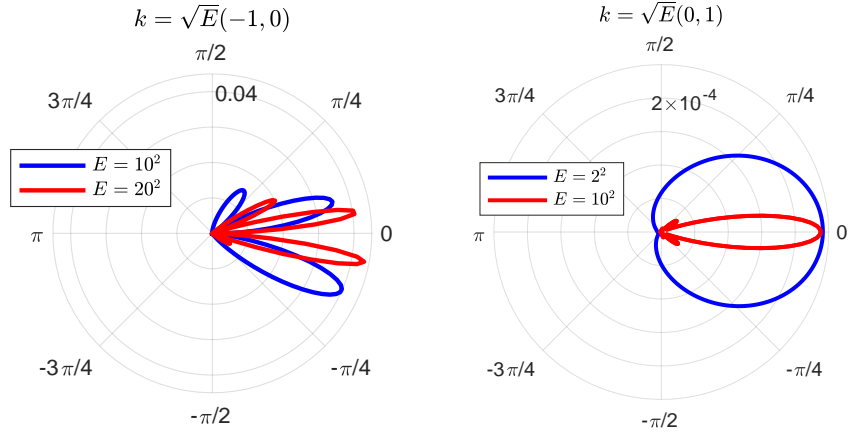


Figure 4: Differential scattering cross-sections $|f(k, l)|^2$ for the potential of Fig. 3 (a) at $k = \sqrt{E}(-1, 0)$ (left) and for the potential of Fig. 6 (a) at $k = \sqrt{E}(0, 1)$ (right). The distance to the curve in direction l is equal to $|f(k, l)|^2$.

the potential in Fig. 3 with $E = 15^2$ the average pointwise noise level $\|\underline{F} - \underline{F}^\dagger\|_2 / \|\underline{F}^\dagger\|_2$ was about 44%, 14%, 4.4% and 1.4% for total count numbers $N_p \in \{10^7, 10^8, 10^9, 10^{10}\}$. However, we stress that pointwise noise levels, although frequently used, are misleading as they tend to infinity as the discretization of the data space becomes finer and finer without loss of information, and that N_p (or $N_p^{-1/2}$) is a better characterization of the noise level.

As the proposed method only yields an approximate solution at fixed energy even for noiseless data, a natural question is how much the reconstructions of our method can be improved by iterative regularization methods. Here we choose the Newton conjugate gradient method (NewtonCG) (see [14]) with H^1 inner product in the preimage space as a commonly used representative of this class of methods, and use the results of our method as starting point of NewtonCG. The stopping index of the NewtonCG iteration was chosen by the discrepancy principle using the estimated noise level $\mathbf{E}\|\underline{F} - \underline{F}^\dagger\|_2^2 = \sum_{l,m} \mathbf{Var}(\underline{F}_l)_m = \sum_{l,m} t_l(k_m)^{-1} (\underline{F}_l^\dagger)_m \approx t_l(k_m)^{-1} (\underline{F}_l)_m$ (even though the discrepancy principle is actually only justified for deterministic noise models, see [14]).

The number of iterations J is chosen basing on the following observations: for small particle count such as $N_p = 10^7$ after two or three iterations the accumulated noise in reconstruction by our method is already comparable with the reconstruction error and the method should be stopped; for bigger particle counts such as $N_p \geq 10^{10}$ the number of steps can be chosen in a relatively large range without significant impact on the reconstruction error; we use $J = 8$ iterations for large particle counts $N_p \geq 10^8$.

Figure 5 shows cross-sections of the reconstructed potentials for the reconstructions using (a) the phaseless Born approximation, (b) our method and (c) our method combined with NewtonCG. In this experiment we used the values of parameters $E = 10^2$ and $N_p = 10^9$ and the highest possible scaling factor for the potential shown in Fig. 3 (a), for which our method still works at this energy level. This corresponds to (L^1, L^2, L^∞) norms (13.5, 14.3, 37.0), respectively.

Table 1 shows the reconstruction errors using the same methods for different energy levels and different expected count numbers N_p . Errors are averaged over 5 experiments. These results demonstrate that our method performs well far beyond the scope of validity of the Born approximation. It can also be seen from these tables that the best reconstruction results are achieved by combining the proposed method with an iterative regularization method such as NewtonCG.

Comparison of convergence regions with NewtonCG. We also studied the influence of scaling of background potentials on reconstructions using our method and using NewtonCG. We made tests for the unknown potential of Fig. 3 (a) and three type-B potentials based on the Wendland functions with $k = 1$.

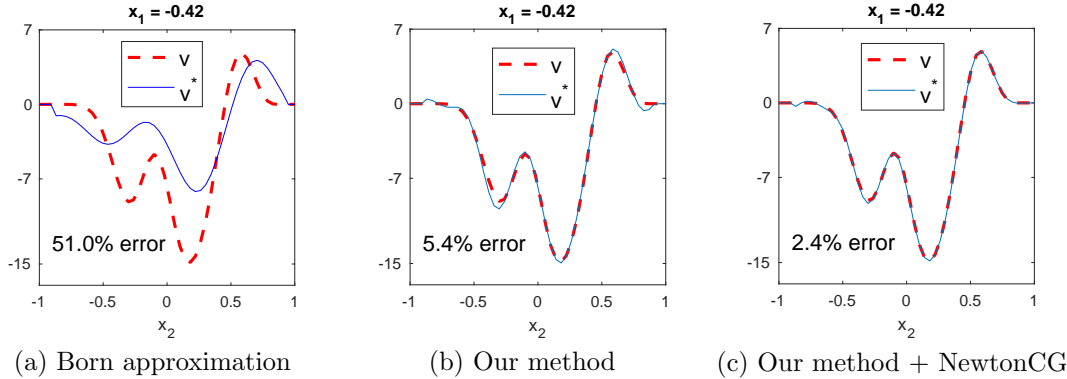


Figure 5: Cross-sections of the exact v and reconstructed potentials v^* , and L^∞ relative reconstruction errors. Here $E = 10^2$ and $N_p = 10^9$.

$N_p \backslash E$	10^2	15^2	20^2	$N_p \backslash E$	10^2	15^2	20^2	$N_p \backslash E$	10^2	15^2	20^2
10^7	53	20	16	10^7	15	8.3	7.9	10^7	6	3.6	5.2
10^8	53	19	16	10^8	7.9	3.2	2.9	10^8	3.8	2	2.4
10^9	53	19	16	10^9	6	1.2	1.3	10^9	2.5	0.95	0.97
10^{10}	53	20	16	10^{10}	5.8	1.1	0.78	10^{10}	2	0.67	0.64

Table 1: relative L^∞ reconstruction errors in percents for the potential v and the background potentials w_1, w_2, w_3 shown in Fig. 3.

First, we tried to recover the potential using NewtonCG with zero initial guess. Simulations show that the iterations do not converge to the exact potentials unless the potential is downscaled by a factor of 75 or bigger. On the other hand, our method works reasonably well, see Tab. 2, column 3B(W), and it can provide an initial guess from which NewtonCG converges.

We also noticed that the simultaneous downscaling of the unknown and background potentials, even by a factor of 1000, does not solve the convergence problem of NewtonCG: the norm ratio of the background potential to the unknown potential must be also sufficiently small to guarantee the convergence of NewtonCG from the zero initial guess.

Non-smooth potentials. Consider the potential of 6 (a). The differential scattering cross-sections of this potential at energies $E = 2^2$ and $E = 10^2$ for the incident direction $k = \sqrt{E}(0, 1)$ is shown at Fig. 4 (right).

Fig. 6 (b), (c) shows reconstructions of this non-smooth potential using the Born approximation and our method without NewtonCG. In the experiment we use background potentials w_1, w_2 of type A (i.e. $w_2 = iw_1$), the energy is $E = 10^2$, and the particle count is $N_p = 10^{15}$. One can see that even though our method is theoretically justified only for sufficiently smooth potentials, it performs well also for non-smooth potentials.

Choice of background potentials. Examples of functions with compact support satisfying assumption (3.6) are Wendland's radial basis functions (see [32]), in particular

$$w(x) = \Phi_k(|x|_2/h) \quad \text{for some } h > 0, k \in \{0, 1\} \text{ and} \quad (4.7)$$

$$\Phi_0(r) := \max(1 - r, 0)^2, \quad \Phi_1(r) := \max(1 - r, 0)^4(4r + 1). \quad (4.8)$$

More precisely, (3.6) is satisfied with $\sigma = d + 2k + 1$ (see [33]), and $w \in C^{2k}(\mathbb{R}^d)$.

We also checked to which extent our approach still works if we use background potentials which do not satisfy assumption (3.6), but may be easier to realize experimentally, such as indicator

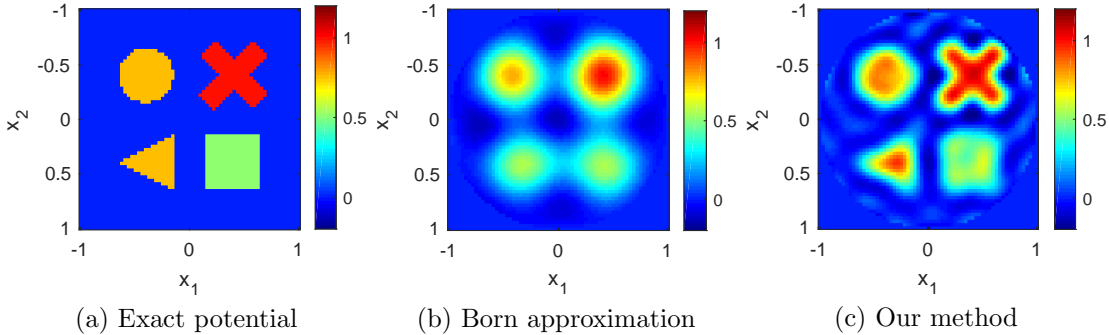


Figure 6: Reconstruction of a non-smooth potential for rectangular background potentials of type A, $E = 10^2$, and $N_p = 10^{15}$.

	2A(R)	2A(W)	3B(R)	3B(W)	2B(R)	2B(W)
Born approximation	20	20	19	21	20	25
our method	2.2	3.4	1.2	5.8	6.5	16
our method+NewtonCG	0.95	1.9	0.95	2.3	2	4.4

Table 2: relative L^∞ reconstruction errors in percents for different choices of background potentials. 2A means two background potentials of type A, whereas 2B and 3B refers to two or three background potentials of type B, respectively. (R) refers to indicator functions of rectangles as in Fig. 3, whereas (W) refers to Wendland functions (4.7) with $k = 1$ with similar scaling. All simulations are performed for $E = 15^2$ and $N_p = 10^9$.

functions of squares. Our results are documented in Table 2 and Fig. 7. It can be seen that non-smooth background potentials yield better results than smooth background potential, but our method still works reasonably well for the C^2 -Wendland function in (4.7). Moreover, the best results are obtained for the nonsmooth rectangular potentials even though they do not satisfy assumption (3.6).

Furthermore, our method yields good results for two background potentials of type A, but significantly worse results for two background potentials of type B. However, the results for type B background potentials can be improved to a quality comparable to type A potentials if either a subsequent NewtonCG iteration is used or if data from a third shifted potential are available.

Robustness against errors in background potentials. In practice it is usually not possible to measure the background potentials exactly. Therefore, we tested our algorithm in the case where the simulated data are generated using a potential \tilde{w} which is a perturbation of the potential w used in our reconstruction method. Figure 8 shows cross-sections of the potentials w and \tilde{w} , and a cross-section of the reconstruction of v . In this example the potential \tilde{w} is obtained from w by amplitude scaling ($\times 1.3$), support scaling ($\times 0.8$), translation by $(0.1, 0)$, addition of Gaussian noise with standard deviation .22 and convolution with Gaussian kernel with standard deviation 0.5. We use the same unknown potential v of Figure 3 as before and set $E = 15^2$, $N_p = 10^9$.

In this example the phaseless Born approximation, our method and our method combined with NewtonCG give the relative L^∞ errors (64%, 3.9%, 1.5%), respectively. This demonstrates a remarkable robustness of our method against errors in the reference potentials.

5 Conclusions

We have proposed a method for the solution of phaseless inverse medium scattering problems in the presence of known background potentials. Let us summarize the advantages and disadvantages

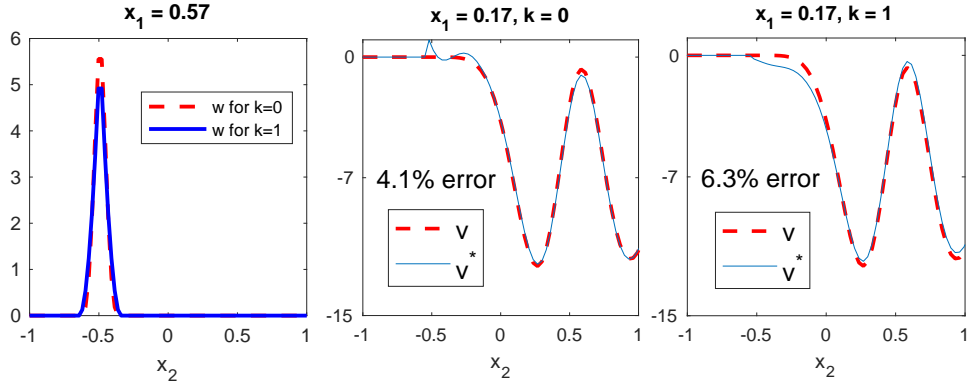


Figure 7: Background potentials based on the Wendland functions Φ_0, Φ_1 defined in (4.7) (left), cross-sections of the unknown potential v and its reconstructions v^* using our method for three type-B background potentials based on Φ_0 (center) and for three type-B background potentials based on Φ_1 (right)

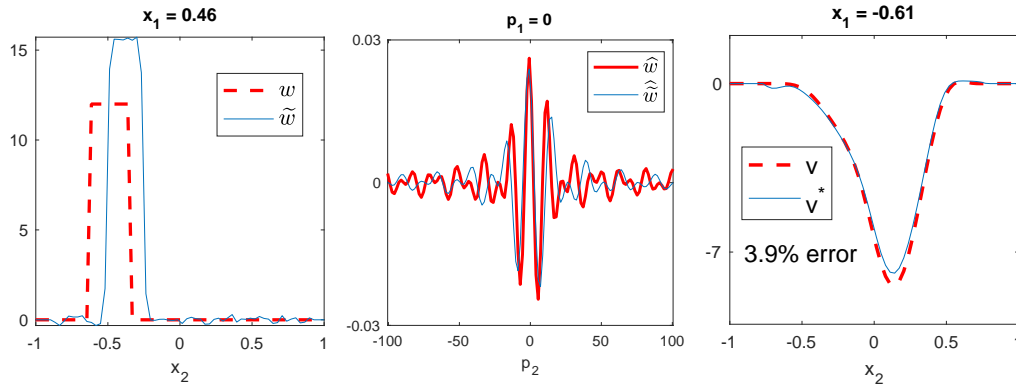


Figure 8: Left and center: Cross-sections of the background potential w used in the reconstruction method and the background potential \tilde{w} used to generate simulated data: (left) space domain; (center) Fourier domain. Right: Cross-sections of the unknown potential v and the potential v^* recovered by our method.

of our method in comparison with iterative regularization methods such as NewtonCG:

- *Global convergence:* Iterative regularization methods require a good initial approximation to the unknown potential, whereas we have shown global convergence of our method as the energy tends to infinity. Numerical experiments at fixed energy demonstrate excellent performance of our method for large potentials and/or weak background potentials where NewtonCG failed.
- *Computation time.* Each iteration step of our reconstruction method requires only $(L + 1)$ solutions of a forward problem, where L is the number of background potentials, and other comparatively cheap operations. In contrast, regularized Newton methods additionally require the solution of a linearized inverse problem in each iteration step, and they typically need a larger number of iteration to achieve the accuracy of our method. In our experiments the proposed method was typically more than 20 times faster than NewtonCG, but we stress that the quotient of computation times strongly depends on the noise level, the energy, the potentials, the choice of the direct solver (setup time vs. solution time), and other parameters.
- *Use of black-box solvers.* As our method only requires the solution of forward scattering

problems, any block-box solver for such problems can be used. In contrast, iterative regularization methods additionally use the Fréchet derivative of the forward operator and typically also the adjoint of the Fréchet derivative. The implementation of these operations may require modifications of the source code of the forward solver.

- *Asymptotic exactness.* At fixed energy in the absence of noise the NewtonCG is expected to converge to the exact solution under some additional assumptions, in particular the uniqueness of solution and the tangential cone condition, see [14]. In contrast, theoretically our method will converge to the exact potential only in the limit $E \rightarrow +\infty$.
- *Stopping rules.* There exists a considerable literature on a-posteriori stopping rules for iterative regularization methods and their convergence properties such as the discrepancy principle for NewtonCG (see [14]). In contrast, we have used a rather ad-hoc a-priori stopping rule in our experiments with the proposed method for the lack of a better alternative.

This discussion shows that the pros and cons of our method are rather complementary to those of iterative regularization methods. Therefore, the proposed method provides a valuable new tool for the solution of phaseless inverse medium scattering problems. Hybrid methods using the proposed method to compute an initial guess for an iterative regularization method allow to combine the advantages of both methods. But in many cases the proposed method itself may already provide a sufficiently accurate reconstruction.

On the theoretical side we have demonstrated fast convergence of our method as energy tends to infinity for exact data and two types of background potentials. It remains for future research to study the behavior of the proposed method in the presence of noise and to devise and analyze useful stopping rules.

A Proofs

A.1 Proof of Lemma 3.1

Under the assumptions of Lemma 3.1, the following estimates hold:

$$\begin{aligned} & \left| |\Phi f_E(p) + \Phi f_{E,j}^*(p) - \Phi f_E(p)| - |\Phi f_{E,j}(p)| \right| \leq \mu_{1,\S A.1} E^{-\alpha-\frac{1}{2}}, \\ & p \in \mathcal{B}_{2\sqrt{E}}^d, E \geq E^*, j = 1, 2, \end{aligned} \quad (\text{A.1})$$

where $\mu_{1,\S A.1} > 0$. The proof of estimates (A.1) is based on the following inequalities:

$$\begin{aligned} & \left| |\Phi f_E + \Phi f_{E,l}^* - \Phi f_E^*| - |\Phi f_{E,j}| \right| \leq |\Phi f_E + \Phi f_{E,l}^* - \Phi f_E^* - \Phi f_{E,l}| \\ & = \left| (\Phi f_E - \widehat{v}) - (\Phi f_E^* - \widehat{v}_E^*) - ((\Phi f_{E,l} - \widehat{v}_{E,l}) - (\Phi f_{E,l}^* - \widehat{v}_{E,l}^*)) \right| \\ & \leq \left| (\Phi f_E - \widehat{v}) - (\Phi f_E^* - \widehat{v}_E^*) \right| + \left| (\Phi f_{E,l} - \widehat{v}_l) - (\Phi f_{E,l}^* - \widehat{v}_{E,l}^*) \right| \end{aligned} \quad (\text{A.2})$$

for $l = 1, 2$. Applying Lemma 2.1 to v, v_E^* and to $v_l, v_{E,l}^*$, respectively, we get the estimates

$$\begin{aligned} & \left| (\Phi f_E(p) - \widehat{v}(p)) - (\Phi f_E^*(p) - \widehat{v}_E^*(p)) \right| \leq \frac{1}{2} \mu_{1,\S A.1} E^{-\alpha-\frac{1}{2}}, \\ & \left| (\Phi f_{E,l}(p) - \widehat{v}_l(p)) - (\Phi f_{E,l}^*(p) - \widehat{v}_{E,l}^*(p)) \right| \leq \frac{1}{2} \mu_{1,\S A.1} E^{-\alpha-\frac{1}{2}}, \quad l = 1, 2, \end{aligned} \quad (\text{A.3})$$

where $\frac{1}{2} \mu_{1,\S A.1} > 0$ is the constant in the right-hand side of formula (3.14) of [28], $p \in \mathcal{B}_{2\sqrt{E}}^d$, $E \geq E^*$. Formula (A.1) follows from (A.2), (A.3).

Next, using (A.1) we get the following estimate:

$$\begin{aligned} & \left| |\Phi f_E(p) + \Phi f_{E,l}^*(p) - \Phi f_E^*(p)|^2 - |\Phi f_{E,l}(p)|^2 \right| \leq \mu_{1,\S A.1} \mu_{2,\S A.1} E^{-\alpha-\frac{1}{2}}, \\ & p \in \mathcal{B}_{2\sqrt{E}}^d, E \geq E^*, l = 1, 2, \end{aligned} \quad (\text{A.4})$$

for $\mu_{2,\S A.1}$ such that

$$\max\{|\Phi f_E|, |\Phi f_{E,1}|, |\Phi f_{E,2}|, |\Phi f_{E,1}^* - \Phi f_E^*|, |\Phi f_{E,2}^* - \Phi f_E^*|\} \leq \frac{1}{3}\mu_{2,\S A.1}, \quad (\text{A.5})$$

where $p \in \mathcal{B}_{2\sqrt{E}}^d$, $E \geq E^*$. The estimate (A.4) can be rewritten as

$$\begin{aligned} & |2\operatorname{Re}(\Phi f_{E,l}^* - \Phi f_E^*) \operatorname{Re} \Phi f_E(p) + 2\operatorname{Im}(\Phi f_{E,l}^* - \Phi f_E^*) \operatorname{Im} \Phi f_E(p) \\ & - (|\Phi f_{E,l}^*|^2 - |\Phi f_E^*|^2 - |\Phi f_{E,l}^* - \Phi f_E^*|^2)| \leq \mu_{1,\S A.1} \mu_{2,\S A.1} E^{-\alpha - \frac{1}{2}}, \quad l = 1, 2. \end{aligned} \quad (\text{A.6})$$

In turn, one can rewrite (A.6) in matrix form as

$$\left| 2M(p, E) \cdot \begin{pmatrix} \operatorname{Re} \Phi f_E(p) \\ \operatorname{Im} \Phi f_E(p) \end{pmatrix} - b(p, E) \right| \leq \mu_{1,\S A.1} \mu_{2,\S A.1} E^{-\alpha - \frac{1}{2}} \quad (\text{A.7})$$

with the matrix M and the vector b from Algorithm 1. Using (3.21), (3.23) and (3.26), we obtain the estimate (3.24).

Using the formula for the inverse matrix, we also get the following equality:

$$\|M^{-1}(p, E)\|_F = \frac{(|\Phi f_{E,1}^* - \Phi f_E^*|^2 + |\Phi f_{E,2}^* - \Phi f_E^*|^2)^{\frac{1}{2}}}{|\zeta^*(p, E)|}, \quad E \geq E^{**}, \quad (\text{A.8})$$

for $p \in \mathcal{B}_{2\sqrt{E}}^d$ such that (3.23) holds and where $\|\cdot\|_F$ denotes the Frobenius matrix norm:

$$\|A\|_F = \sqrt{\sum_{i,j=1}^n |a_{ij}|^2} \quad \text{for any square matrix } A = (a_{ij})_{i,j=1}^n.$$

Using (3.24), (A.5), (A.8) we obtain the estimate

$$\|M^{-1}(p, E)\|_F \leq \frac{2\sqrt{2}}{3}\delta^{-1}\mu_{2,\S A.1}, \quad E \geq E^{**}. \quad (\text{A.9})$$

Finally, using (A.7) and (A.9), we get the estimate (3.25), where

$$\mu_{3,\S 3.2} = \frac{2}{3}\mu_{1,\S A.1}\mu_{2,\S A.1}^2. \quad (\text{A.10})$$

Lemma 3.1 is proved.

A.2 Proof of Theorem 3.2

Proposition A.1. *Let v and w_1, w_2 be the same as in (1.1b), (3.6), (3.8). Let v_E^* be an approximation to v satisfying (2.12). Let $U_E^{**}(p)$ be defined according to (3.27), Then*

$$\begin{aligned} |U_E^{**}(p) - \widehat{v}(p)| &\leq \mu_{1,\S A.2} E^{-\alpha - \frac{1}{2}} r^{2\sigma}, \quad \mu_{1,\S A.2} := 4^\sigma \mu_{1,\S 3.1}^{-2} \mu_{3,\S 3.2} + \mu_{1,\S 2.2}, \\ E &\geq \max\{\mu_{2,\S A.2} r^{4\sigma}, E^*\}, \quad \mu_{2,\S A.2} := 4^{2\sigma+1} \mu_{1,\S 3.1}^{-4} \mu_{1,\S 3.2}^2, \\ p &\in \mathcal{B}_r^d, \quad 1 \leq r \leq 2\sqrt{E}, \end{aligned} \quad (\text{A.11})$$

where σ is the same as in (3.6), $E^* = E^*(K, D_{\text{ext}})$ is defined according to (2.13), (3.17), and $\mu_{k,\S X}$, $k \geq 1$, are the constants of Section X.

Proof of Proposition A.1. Due to (2.13), (3.27) and Lemma 3.1, we have

$$\begin{aligned} |U_E^{**}(p) - \widehat{v}(p)| &\leq (\mu_{3,\S 3.2} \delta^{-1} + \mu_{1,\S 2.2}) E^{-\alpha - \frac{1}{2}}, \\ \text{if } p &\in \mathcal{B}_{2\sqrt{E}}^d, \quad |\zeta_{\widehat{w}_1, \widehat{w}_2}(p)| \geq \delta, \quad E \geq E^{**}, \\ E^{**} &= \max(4\mu_{1,\S 3.2}^2 \delta^{-2}, E^*). \end{aligned} \quad (\text{A.12})$$

Besides, in view of (3.9), we also have that

$$\min_{p \in \mathcal{B}_r^d} |\zeta_{\widehat{w}_1, \widehat{w}_2}(p)| = \mu_{1,\S 3.1}^2 (1+r)^{-2\sigma} \geq \mu_{1,\S 3.1}^2 4^{-\sigma} r^{-2\sigma}, \quad 1 \leq r. \quad (\text{A.13})$$

Using (A.12) with $\delta = \mu_{1,\S 3.1}^2 4^{-\sigma} r^{-2\sigma}$ and (A.13), we get (A.11). \square

We represent v as follows:

$$\begin{aligned} v(x) &= v^+(x, r) + v^-(x, r), \quad x \in \mathbb{R}^d, r > 0, \\ v^+(x, r) &= \int_{\mathcal{B}_r^d} e^{-ipx} \widehat{v}(p) dp, \\ v^-(x, r) &= \int_{\mathbb{R}^d \setminus \mathcal{B}_r^d} e^{-ipx} \widehat{v}(p) dp. \end{aligned} \tag{A.14}$$

Since $v \in W^{n,1}(\mathbb{R}^d)$, $n > d$, we have

$$\begin{aligned} |v^-(x, r)| &\leq \mu_{3,\S A.2} \|v\|_{n,1} r^{d-n}, \quad x \in \mathbb{R}^d, r > 0, \\ \mu_{3,\S A.2} &:= |\mathbb{S}^{d-1}| \frac{(2\pi)^{-d} d^n}{n-d}, \end{aligned} \tag{A.15}$$

where $\|\cdot\|_{n,1}$ is defined in (2.7), and $|\mathbb{S}^{d-1}|$ is the standard Euclidean volume of \mathbb{S}^{d-1} ; see [1].

Using (A.11) we obtain

$$\begin{aligned} \left| v^+(x, r) - \int_{\mathcal{B}_r^d} e^{-ipx} U_{\widehat{w}_1, \widehat{w}_2}(p, E) dp \right| &\leq \mu_{1,\S A.2} |\mathcal{B}_1^d| E^{-\alpha - \frac{1}{2}} r^{d+2\sigma} \\ \text{for } x \in D, 1 \leq r \leq 2\sqrt{E}, E &\geq \max\{\mu_{2,\S A.2} r^{4\sigma}, E^*\}, \end{aligned} \tag{A.16}$$

where $|\mathcal{B}_1^d|$ denotes the standard Euclidean volume of \mathcal{B}_1^d .

It follows from (A.14), (A.15), and (A.16) that

$$\begin{aligned} \left| v(x) - \int_{\mathcal{B}_r^d} e^{-ipx} U_{\widehat{w}_1, \widehat{w}_2}(p, E) dp \right| &\leq \mu_{3,\S A.2} \|v\|_{n,1} r^{d-n} + \mu_{1,\S A.2} |\mathcal{B}_1^d| E^{-\alpha - \frac{1}{2}} r^{d+2\sigma} \\ \text{for } x \in D, 1 \leq r \leq 2\sqrt{E}, E &\geq \max\{\mu_{2,\S A.2} r^{4\sigma}, E^*\}. \end{aligned} \tag{A.17}$$

In addition, if $r = r(E)$, where $r(E)$ is the radius of (3.29), then

$$\begin{aligned} r^{d-n} &= (2\tau)^{d-n} E^{-\beta}, \\ E^{-\alpha - \frac{1}{2}} r^{d+2\sigma} &= (2\tau)^{d+2\sigma} E^{-\beta}, \end{aligned} \tag{A.18}$$

$$\begin{aligned} E &\geq \mu_{2,\S A.2} r(E)^{4\sigma} \quad \text{if } E \geq \mu_{4,\S A.2}, \\ \mu_{4,\S A.2} &:= (\mu_{2,\S A.2} (2\tau)^{4\sigma})^{\frac{n-d}{n-d-4\beta\sigma}}. \end{aligned} \tag{A.19}$$

Using formulas (3.29), (A.17), (A.18), (A.19), we obtain

$$\begin{aligned} |v_E^{**}(x) - v(x)| &\leq B_1 E^{-\beta} \quad \text{for } x \in D, E \geq E_1 \quad \text{with} \\ B_1 &:= (2\tau)^{d-n} \mu_{3,\S A.2} \|v\|_{n,1} + (2\tau)^{d+2\sigma} \mu_{1,\S A.2} |\mathcal{B}_1^d|, \\ E_1 &:= \max\{\mu_{4,\S A.2}, E^*\}. \end{aligned} \tag{A.20}$$

Theorem 3.2 is proved.

Remark A.2. We have that

$$E_1 = E^* \quad \text{for } \tau \leq \tau_1 \quad \text{for } \tau_1 := \frac{1}{2} \mu_{2,\S A.2}^{-\frac{1}{4\sigma}} (E^*)^{1 - \frac{4\beta\sigma}{n-d}}. \tag{A.21}$$

A.3 Proof of Theorem 3.5

Proposition A.3. Let v satisfy (1.1b) and $v \in W^{n,1}(\mathbb{R}^d)$. Let $y \in \mathbb{R}^d$, $y \neq 0$, and $N \geq 1$. Put

$$\begin{aligned} V^{N,\varepsilon}(p^\varepsilon(p_\perp, z, t)) &= \sum_{-N \leq j \leq N, j \neq 0} \widehat{v}(p^\varepsilon(p_\perp, z, j)) L_j(t), \\ p_\perp &\in \mathbb{R}^d, p_\perp \cdot y = 0, z \in \mathbb{Z}, t \in (-1, 1), 0 < \varepsilon < \min\{\frac{1}{2}|y|, \frac{\pi}{N+1}\}, \end{aligned} \tag{A.22}$$

where $p^\varepsilon(p_\perp, z, t)$, L_j are defined in (3.36), (3.40). Then

$$\begin{aligned} |V^{N,\varepsilon}(p) - \widehat{v}(p)| &\leq \mu_{1,\S A.3} \varepsilon^{2N} (1 + |p_\perp| + \frac{\pi}{|y|} |z|)^{-n}, \\ p &= p^\varepsilon(p_\perp, z, t), \quad p_\perp \in \mathbb{R}^d, \quad p_\perp \cdot y = 0, \quad z \in \mathbb{Z}, \quad t \in (-1, 1), \\ \mu_{1,\S A.3} &:= \frac{2^{n-d}}{\pi^d} (1+d)^n \frac{(2N)^{2N}}{(2N)!|y|^{4N}} \|(x \cdot y)^{2N} v(x)\|_{n,1}. \end{aligned} \quad (\text{A.23})$$

Proof of Proposition A.3. Let $p_\perp \in \mathbb{R}^d$, $p_\perp \cdot y = 0$ and $z \in \mathbb{Z}$ be fixed. The following estimate holds:

$$\begin{aligned} |V^{N,\varepsilon}(p) - \widehat{v}(p)| &\leq \frac{(2N)^{2N}}{(2N)!|y|^{4N}} \varepsilon^{2N} \sup_{s \in [-N, N]} |([y\nabla]^{2N} \widehat{v})(p^\varepsilon(p_\perp, z, s))|, \\ p &= p^\varepsilon(p_\perp, z, t), \quad t \in (-1, 1), \quad (y\nabla\varphi)(\xi) = y_1 \frac{\partial\varphi(\xi)}{\partial\xi_1} + \dots + y_d \frac{\partial\varphi(\xi)}{\partial\xi_d}. \end{aligned} \quad (\text{A.24})$$

Estimate (A.24) follows from the formula

$$\frac{\partial}{\partial s} p^\varepsilon(p_\perp, z, s) = \varepsilon \frac{y}{|y|^2}, \quad (\text{A.25})$$

from the fact that $P(t) = V^{N,\varepsilon}(p^\varepsilon(p_\perp, z, t))$ in the Lagrange interpolating polynomial for $u(t) = \widehat{v}(p^\varepsilon(p_\perp, z, t))$ with the nodes at $t = \pm 1, \dots, \pm N$, and from the following standard estimate for the Lagrange interpolating polynomial $P(t) = V^{N,\varepsilon}(p^\varepsilon(p_\perp, z, t))$:

$$\begin{aligned} |V^{N,\varepsilon}(p) - \widehat{v}(p)| &\leq \frac{(2N)^{2N}}{(2N)!} \sup_{s \in [-N, N]} \left| \frac{\partial^{2N}}{\partial s^{2N}} \widehat{v}(p^\varepsilon(p_\perp, z, s)) \right|, \\ p &= p^\varepsilon(p_\perp, z, t), \quad t \in [-N, N]. \end{aligned} \quad (\text{A.26})$$

In addition, the following estimate was proved in [1]:

$$(1 + |p|)^n |\widehat{v}(p)| \leq (2\pi)^{-d} (1+d)^n \|v(x)\|_{n,1}, \quad p \in \mathbb{R}^d. \quad (\text{A.27})$$

If we replace $v(x)$ by $(x \cdot y)^{2N} v(x)$, we get

$$(1 + |p|)^n |[y\nabla]^{2N} \widehat{v}(p)| \leq (2\pi)^{-d} (1+d)^n \|(x \cdot y)^{2N} v(x)\|_{n,1}, \quad p \in \mathbb{R}^d. \quad (\text{A.28})$$

Besides, we also have that

$$1 + |p| \geq \frac{1}{2} (1 + |p_\perp| + \frac{\pi}{|y|} |z(p)|), \quad p \in Z_y^\varepsilon, \quad (\text{A.29})$$

where we have used that $\varepsilon < \frac{1}{2}|y|$. Using (A.24), (A.28), (A.29), we get (A.23).

Proposition A.3 is proved. \square

Proposition A.4. Let v and w_1, w_2 be the same as in (1.1b), (3.6), (3.8). Let v_E^* be an approximation to v satisfying (2.12). Let U_E^{**} be defined according to (3.27), and let $U_{N,\varepsilon}^*(p, E)$ be defined according to (3.36), (3.38), (3.39), (3.40). Then

$$|\widehat{v}(p) - U_E^{**}(p)| \leq \mu_{2,\S A.3} E^{-\alpha - \frac{1}{2}} r^{2\sigma} \varepsilon^{-1}, \quad \mu_{2,\S A.3} := 4^\sigma \frac{\pi}{2} \mu_{1,\S 3.1}^{-2} \mu_{3,\S 3.2} + \mu_{1,\S 2.2}, \quad (\text{A.30})$$

$$\text{for } p \in \mathcal{B}_r^d \setminus Z_y^\varepsilon, \quad 0 < \varepsilon < 1, \quad 1 \leq r \leq 2\sqrt{E}, \quad (\text{A.31})$$

$$E \geq \max(\mu_{3,\S A.3} r^{4\sigma} \varepsilon^{-2}, E^*), \quad \mu_{3,\S A.3} := 4^{2\sigma} \pi^2 \mu_{1,\S 3.1}^{-4} \mu_{1,\S 3.2}^2,$$

where σ is the same as in (3.6), $E^* = E^*(K, D_{ext})$ is defined according to (2.13), (3.17), and $\mu_{k,\S X}$, $k \geq 1$, are the constants of Section X.

In addition, if $v \in W^{n,1}(\mathbb{R}^d)$, $n \geq 0$, then

$$|\widehat{v}(p) - U_{N,\varepsilon}^{**}(p, E)| \leq \mu_{4,\S A.3} E^{-\alpha - \frac{1}{2}} r^{2\sigma} \varepsilon^{-1} + \mu_{1,\S A.3} \varepsilon^{2N} (1 + |p_\perp| + \frac{\pi}{|y|} |z|)^{-n}, \quad (\text{A.32})$$

$$\mu_{4,\S A.3} := 4^{\sigma+1} \max(1, \frac{\pi}{|y|})^{2\sigma} N (1 - (\frac{N}{N+1})^N) \mu_{2,\S A.3},$$

$$\text{for } p = p^\varepsilon(p_\perp, z, t) \in \mathcal{B}_r^d \cap Z_y^\varepsilon, \quad 0 < \varepsilon < \min\{1, \frac{1}{2}|y|, \frac{\pi}{N+1}\}, \quad (\text{A.33})$$

$$1 \leq r \leq 2\sqrt{E} - \frac{\pi}{|y|}, \quad E \geq \max(\mu_{3,\S A.3} r^{4\sigma} \varepsilon^{-2}, E^*).$$

Proof of Proposition A.4. As in the proof of Proposition A.1, we have formula (A.12).

Besides, it follows from (3.7) that

$$\begin{aligned} |\zeta_{\widehat{w}_1, \widehat{w}_2}(p)| &\geq 4^{-\sigma} \frac{2}{\pi} \mu_{1, \S 3.1}^2 r^{-2\sigma} \varepsilon, \\ p &\in \mathcal{B}_r^d \setminus Z_y^\varepsilon, \quad 0 < \varepsilon < 1, \quad 1 \leq r \leq 2\sqrt{E}. \end{aligned} \quad (\text{A.34})$$

Using (A.34) and (A.12) with $\delta = 4^{-\sigma} \frac{2}{\pi} (\mu_{1, \S 3.1})^2 r^{-2\sigma} \varepsilon$, we get (A.30).

It remains to prove (A.32). Using definition (3.38), one can write

$$\begin{aligned} U_{N, \varepsilon}^{**}(p, E) - \widehat{v}(p) &= \varphi^{N, \varepsilon}(p, E) + V^{N, \varepsilon}(p), \\ \text{for } p = p^\varepsilon(p_\perp, z, t) &\in \mathcal{B}_r^d \cap Z_y^\varepsilon, \quad r \leq 2\sqrt{E} - \frac{\pi}{|y|} \text{ with} \\ \varphi^{N, \varepsilon}(p, E) &:= \sum_{-N \leq j \leq N, j \neq 0} [U^{**}(p^\varepsilon(p_\perp, z, j), E) - \widehat{v}(p^\varepsilon(p_\perp, z, j))] L_j(t), \end{aligned} \quad (\text{A.35})$$

where $V^{N, \varepsilon}$ is given by (A.22).

Using estimate (A.30) and formulas (3.38), (3.42), (A.35) we get

$$\begin{aligned} |\varphi^{N, \varepsilon}(p, E)| &\leq \mu_{2, \S A.3} E^{-\alpha - \frac{1}{2}} \left(r + \frac{\pi}{|y|}\right)^{2\sigma} \varepsilon^{-1} \sum_{-N \leq j \leq N, j \neq 0} |L_j(t)| \\ &\leq 4^\sigma \max(1, \frac{\pi}{|y|})^{2\sigma} \mu_{2, \S A.3} E^{-\alpha - \frac{1}{2}} \varepsilon^{-1} r^{2\sigma} \sum_{-N \leq j \leq N, j \neq 0} |L_j(t)|, \\ p = p^\varepsilon(p_\perp, z, t) &\in \mathcal{B}_r^d \cap Z_y^\varepsilon, \quad 1 \leq r \leq 2\sqrt{E} - \frac{\pi}{|y|}. \end{aligned} \quad (\text{A.36})$$

Note that for $t \in (-1, 1)$ and $j = \pm 1, \dots, \pm N$,

$$\begin{aligned} |L_j(t)| &= \frac{|j||t+j|}{(N-j)!(N+j)!} \prod_{1 \leq i \leq N, i \neq j} (i^2 - t^2) \\ &\leq \frac{2N!N!}{(N-j)!(N+j)!} \leq 2 \left(\frac{N}{N+1}\right)^{|j|}. \end{aligned} \quad (\text{A.37})$$

Consequently,

$$\sum_{-N \leq j \leq N, j \neq 0} |L_j(t)| \leq 4N \left(1 - \left(\frac{N}{N+1}\right)^N\right), \quad t \in (-1, 1). \quad (\text{A.38})$$

Using (A.36), (A.38), we get

$$\begin{aligned} |\varphi^{N, \varepsilon}(p, E)| &\leq \mu_{4, \S A.3} E^{-\alpha - \frac{1}{2}} r^{2\sigma} \varepsilon^{-1}, \\ \text{for } p = p^\varepsilon(p_\perp, z, t) &\in \mathcal{B}_r^d \cap Z_y^\varepsilon, \quad 1 \leq r \leq 2\sqrt{E} - \frac{\pi}{|y|}, \\ E &\geq \max(\mu_{3, \S A.3} r^{4\sigma} \varepsilon^{-2}, E^*). \end{aligned} \quad (\text{A.39})$$

Using (A.23), (A.35), (A.39), we get (A.32).

Proposition A.4 is proved. \square

The final part of the proof of Theorem 3.5 is as follows. In a similar way with (A.14), we represent v as follows:

$$\begin{aligned} v(x) &= v_1^+(x, r) + v_2^+(x, r) + v^-(x, r), \quad x \in D, \quad r > 0 \text{ with} \\ v_1^+(x, r) &:= \int_{\mathcal{B}_r^d \setminus Z_y^\varepsilon} e^{-ipx} \widehat{v}(p) dp, \\ v_2^+(x, r) &:= \int_{\mathcal{B}_r^d \cap Z_y^\varepsilon} e^{-ipx} \widehat{v}(p) dp, \\ v^-(x, r) &:= \int_{\mathbb{R}^d \setminus \mathcal{B}_r^d} e^{-ipx} \widehat{v}(p) dp. \end{aligned} \quad (\text{A.40})$$

Since $v \in W^{n,1}(\mathbb{R}^d)$, estimate (A.15) holds.

Using estimates (A.30), (A.32), we get:

$$\left| v_1^+(x, r) - \int_{\mathcal{B}_r^d \setminus Z_y^\varepsilon} e^{-ipx} U^{**}(p, E) dp + v_2^+(x, r) - \int_{\mathcal{B}_r^d \cap Z_y^\varepsilon} e^{-ipx} U_{N,\varepsilon}^{**}(p, E) dp \right| \leq I_1 + I_2, \quad (\text{A.41})$$

$$I_1 := 2^{2\sigma} \mu_{2,\S A.3} |\mathcal{B}_1^d| E^{-\alpha - \frac{1}{2}} r^{d+2\sigma} \varepsilon^{-1}, \quad (\text{A.42})$$

$$I_2 := \mu_{1,\S A.3} \varepsilon^{2N} \int_{\mathcal{B}_r^d \cap Z_y^\varepsilon} \left(1 + \frac{\pi}{|y|} |z(p)| + |p_\perp|\right)^{-n} dp, \quad (\text{A.43})$$

$$x \in D, \quad 1 \leq r \leq 2\sqrt{E} - \frac{\pi}{|y|}, \quad \text{for } E \text{ as in (A.33)}.$$

In addition, we have the following estimate proved in [1] (see the proof of Theorem 2 of [1]):

$$I_2 \leq \mu_{5,\S A.3} \varepsilon^{2N+1}, \quad \mu_{5,\S A.3} := \mu_{1,\S A.3} \frac{2}{|y|} \frac{|\mathbb{S}^{d-2}|}{n-d+1} \sum_{z \in \mathbb{Z}} \left(1 + \frac{\pi}{|y|} |z|\right)^{d-n-1}. \quad (\text{A.44})$$

In addition, if $r = r(E)$, $\varepsilon = \varepsilon(E)$, where $r(E)$, $\varepsilon(E)$ are defined in (3.44), then

$$\begin{aligned} r^{d-n} &= (2\tau)^{d-n} E^{-\beta}, \\ \varepsilon^{-1} E^{-\alpha - \frac{1}{2}} r^{d+2\sigma} &= (2\tau)^{d+2\sigma} E^{-\beta}, \\ \varepsilon^{2N+1} &= E^{-\beta}. \end{aligned} \quad (\text{A.45})$$

Next, we establish a lower bound for E for which $r = r(E)$, $\varepsilon = \varepsilon(E)$ satisfy conditions (A.31), (A.33) of Proposition A.4. Note that

$$\begin{aligned} E &\geq \mu_{3,\S A.3} r(E)^{4\sigma} \varepsilon(E)^{-2} \quad \text{if } E \geq \mu_{6,\S A.3}, \\ \mu_{6,\S A.3} &:= \left(\mu_{3,\S A.3} (2\tau)^{4\sigma}\right)^{\frac{(n+2\sigma)(2N+1)+n-d}{(n-4\alpha\sigma)(2N+1)-2\alpha(n-d)}}. \end{aligned} \quad (\text{A.46})$$

Besides,

$$r(E) \leq 2\sqrt{E} - \frac{\pi}{|y|} \quad \text{if } E \geq 1. \quad (\text{A.47})$$

In addition,

$$\begin{aligned} \varepsilon(E) &< \min\left\{1, \frac{1}{2}|y|, \frac{\pi}{N+1}\right\} \quad \text{if } E > \mu_{7,\S A.3}, \\ \mu_{7,\S A.3} &:= \left(\max\left\{1, \frac{2}{|y|}, \frac{N+1}{\pi}\right\}\right)^{\frac{2N+1}{\beta}}. \end{aligned} \quad (\text{A.48})$$

Using the representation (A.40) and formulas (3.44), (A.15), (A.41), (A.42), (A.44)–(A.48) we get

$$\begin{aligned} |v_E^{**}(x) - v(x)| &\leq B_2 E^{-\beta} \quad \text{with} \\ B_2 &:= \mu_{3,\S A.2} (2\tau)^{d-n} \|v\|_{n,1} + 2^{2\sigma} \mu_{2,\S A.3} |\mathcal{B}_1^d| (2\tau)^{d+2\sigma} + \mu_{5,\S A.3}, \\ E_2 &:= \max\{\mu_{6,\S A.3}, \mu_{7,\S A.3}, E^*\}. \end{aligned} \quad (\text{A.49})$$

Theorem 3.5 is proved.

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