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Representation of the Potential in the Schrödinger Equation

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Results from the solution of the inverse-scattering problem in three dimensions are used to obtain representations of the potential and of the zero-energy wave function in terms of the scattering amplitude, the bound states, and the positive-energy wave functions. Some simple consequences are derived.

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The solution of the inverse-scattering problem in one dimension has led to a well-known representation[1] of the integral of the potential in terms of the reflection coefficient, the bound states, and the scattering wave function, a representation that may be regarded as the inverse of that of the reflection coefficient in terms of the potential and the wave function.[2] I wish to present here an analogous representation in three dimensions and some of its consequences.

We start with the well-known relation between the scattering wave functions ψ^+ and ψ^-, involving the S matrix:

$$\psi^+(-k,-\theta,\vec{x}) = \psi^-(k,\theta,\vec{x}) = \int d\theta'\, S(-k,-\theta,\theta')\psi^+(k,\theta',\vec{x}). \tag{1}$$

Here $k=(2mE)^{1/2}$ is the wave number, θ is a unit vector in the direction of the momentum, $\vec{x} \in R^3$,

$$S(k,\theta,\theta') = \delta(\theta,\theta') - (k/2\pi i)A(k,\theta,\theta'),$$

where A is the scattering amplitude, and $\psi^{\pm}$ are normalized to approach $\exp(ik\theta\cdot\vec{x})$ as $|\vec{x}|\to\infty$. Defining $\gamma(k,\theta,\vec{x}) \equiv \psi^+(k,\theta,\vec{x})\exp(-ik\theta\cdot\vec{x})$ we may write Eq. (1) in the form

$$\gamma(-k,-\theta,\vec{x}) = \gamma(k,\theta,\vec{x}) - (k/2\pi i)\int d\theta'\, A(-k,\theta,\theta')\nu(k,\theta,\theta',\vec{x}), \tag{2}$$

where

$$\nu(k,\theta,\theta',\vec{x}) \equiv \psi^+(k,\theta',\vec{x})\exp(-ik\theta\cdot\vec{x}).$$

The Fourier transform of $\gamma-1$,

$$\zeta(\alpha,\theta,\vec{x}) = (1/2\pi)\int_{-\infty}^{\infty} dk\, e^{-ik\alpha}[\gamma(k,\theta,\vec{x})-1],$$

therefore satisfies the equation

$$\zeta(\alpha,-\theta,\vec{x}) - \zeta(-\alpha,\theta,\vec{x}) = \frac{i}{(2\pi)^2}\int_{-\infty}^{\infty} dk\, k\int d\theta'\, e^{ik\alpha}A(-k,\theta,\theta')\nu(k,\theta,\theta',\vec{x}). \tag{3}$$

Regarded as a function of k, $\gamma-1$ is in $L^2(-\infty,\infty)$, it is the boundary value of an analytic function meromorphic in C^+, and it tends to zero as $|k|\to\infty$ there.[3] Together with the fact that ψ^+ satisfies the

Schrödinger equation with the potential $V(x)$, these properties lead to the relations[4]

$$\lim_{\alpha\uparrow 0}\zeta(\alpha,\theta,\vec{x})\equiv\zeta(0-)=\sum_{n,b}Y_n^b(-\theta)u_n^b(\vec{x})\exp(\kappa_n\theta\cdot\vec{x})/(2\kappa_n) \tag{4}$$

and

$$V(\vec{x})=-2\theta\cdot\nabla[\zeta(0+,\theta,\vec{x})-\zeta(0-,\theta,\vec{x})]. \tag{5}$$

Here $-\kappa_n^2$ are the bound-state eigenvalues, if any, of $-\Delta+V(\vec{x})$, $u_n^b(\vec{x})$ are the corresponding normalized eigenfunctions, and $Y_n^b(\theta)$ are their characters.[5] In the absence of bound states the right-hand side (rhs) of (4) vanishes. Alternatively,[6]

$$\int_0^\infty dr\, V(\vec{x}-\theta r)=2\zeta(0-,\theta,\vec{x})-2\zeta(0+,\theta,\vec{x}). \tag{5'}$$

The implied independence of the rhs of (5) of the direction θ is the "miracle."[3,4,6]

Insertion of (3) and (4) in (5) yields the representation[7]

$$\begin{aligned}V(\vec{x})=\theta\cdot\nabla\{&(2\pi^2 i)^{-1}\int_{-\infty}^{\infty}dk\,k\int d\theta' A(-k,\theta,\theta')\exp(-ik\theta\cdot\vec{x})\psi^+(k,\theta',\vec{x})\\&+\tfrac{1}{2}\sum_{n,b}\kappa_n^{-1}u_n^b(\vec{x})[Y_n^b(-\theta)\exp(\kappa_n\theta\cdot\vec{x})-Y_n^b(\theta)\exp(-\kappa_n\theta\cdot\vec{x})]\},\end{aligned} \tag{6}$$

which is the three-dimensional generalization of a well-known expansion in one dimension.[1] It may be regarded as an inversion of the familiar formula

$$A(k,\theta,\theta')=-(1/4\pi)\int d^3x\, V(x)\exp(-ik\theta\cdot\vec{x})\psi^+(k,\theta',\vec{x}).$$

Of course, there is an analog of (6) obtained from (5′) rather than (5).

If differentiation under the integral sign is justified, then the Schrödinger equation

$$(\Delta+2ik\theta\cdot\nabla-V)\nu(k,\theta,\theta',\vec{x})=0$$

leads to the equation

$$(\Delta-V)\Gamma=0, \tag{7}$$

where

$$\begin{aligned}\Gamma(\vec{x})\equiv 1+&(2\pi)^{-2}\int_{-\infty}^{\infty}dk\int d\theta' A(-k,\theta,\theta')\nu(k,\theta,\theta',\vec{x})\\&+\tfrac{1}{2}\sum_{n,b}\kappa_n^{-2}u_n^b(\vec{x})[Y_n^b(\theta)\exp(-\kappa_n\theta\cdot\vec{x})+Y_n^b(-\theta)\exp(\kappa_n\theta\cdot\vec{x})].\end{aligned} \tag{8}$$

Since $\Gamma(\vec{x})\to 1$ as $|\vec{x}|\to\infty$, $\Gamma(x)$ equals the zero-energy scattering wave function, $\Gamma(x)=\psi^+(0,\theta,x)=\psi^-(0,\theta,x)$, which is independent of θ.

If we define

$$\phi(k,\theta,\vec{x})\equiv\psi^+(k,\theta,\vec{x})\Lambda(\vec{x}),\quad v_n^b(\vec{x})\equiv u_n^b(\vec{x})\Lambda(\vec{x}),\quad \Lambda(\vec{x})\equiv 1/\Gamma(\vec{x}),$$

then

$$\begin{aligned}\Lambda(\vec{x})=1-&(2\pi)^{-2}\int_{-\infty}^{\infty}dk\int d\theta' A(-k,\theta,\theta')\exp(-ik\theta\cdot\vec{x})\phi(k,\theta',\vec{x})\\&-\tfrac{1}{2}\sum_{n,b}\kappa_n^{-2}v_n^b(x)[Y_n^b(\theta)\exp(-\kappa_n\theta\cdot\vec{x})+Y_n^b(-\theta)\exp(\kappa_n\theta\cdot\vec{x})],\end{aligned} \tag{9}$$

and the Lippmann-Schwinger equation for ϕ reads

$$\phi(k,\theta,\vec{x})=e^{ik\theta\cdot\vec{x}}+(2\pi)^{-1}\int d^3y\frac{e^{ik|\vec{x}-\vec{y}|}}{|\vec{x}-\vec{y}|}[\nabla\ln\Lambda(\vec{y})]\cdot\nabla\phi(k,\theta,\vec{y}). \tag{10}$$

The nonlinear system (9) and (10) may be regarded as an alternative formulation of the inverse-scattering problem.

A simple consequence of the fact that $\Gamma(\vec{x})$ is equal to the zero-energy wave function, and therefore $\int d^3x\, V(x)\Gamma(x)=-4\pi A(0)$, is obtained by multiplying (8) by $V(\vec{x})$ and integrating over all $\vec{x}$. The result is[8]

$$\int_0^\infty dk\,\sigma(k,\theta)=\tfrac{1}{2}\pi\int d^3x\,V(\vec{x})+2\pi^2A(0)+\tfrac{1}{2}\pi\sum_{n,b}\kappa_n^{-2}Y_n^b(\theta)\,Y_n^b(-\theta), \tag{11}$$

where $A(0)=A(0,\theta,\theta')$ is the zero-energy scattering amplitude (which is independent of θ and θ'), and $\sigma(k,\theta)=\int d\theta'|A(k,\theta',\theta)|$ is the total cross section for scattering from the incident direction θ. The sum rule (11) is not new; it can be obtained alternatively as the zero-energy limit of a forward dispersion relation.[9] However, it has a remarkable property that appears to have gone unnoticed:[10] It implies that if there are no bound states then the integral on the lhs must be independent of θ. On the other hand, if V produces bound states then the integral on the lhs generally will depend on θ, as shown by the sum on the rhs. This may be regarded as a directly observable consequence of the "miracle." For central potentials, of course, $\sigma(k,\theta)$ is independent of θ. In that case the characters are spherical harmonics, and the m degeneracy leads to a sum on the rhs that is also independent of θ.

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[1]See, for example, F. Calogero and A. Degasperis, *Spectral Transform and Solitons* (North-Holland, Amsterdam, 1982), p. 21, Eq. (3).

[2]See, for example, F. Calogero and A. Degasperis, *Spectral Transform and Solitons* (North-Holland, Amsterdam, 1982), p. 21, Eq. (7).

[3]R. G. Newton, J. Math. Phys. (N.Y.) **21**, 1698 (1980).

[4]R. G. Newton, J. Math. Phys. (N.Y.) **23**, 594 (1982). Note that the rhs of the equation on line 27 in the left-hand column of p. 597 lacks a factor of $1/2\kappa_m$. We assume that $k=0$ is not an exceptional point.

[5]Section 5 of Ref. 3.

[6]R. G. Newton, in *Conference on Inverse Scattering: Theory and Applications* (SIAM, Philadelphia, 1983), pp. 1–74.

[7]It is easy to show that in (6) it is immaterial whether the integral is taken as the limit of the rhs of (3) as $\alpha\downarrow 0$ or $\alpha\uparrow 0$.

[8]Equation (5.6) of Ref. 3 has been used here.

[9]See, for example, J. R. Taylor, *Scattering Theory* (Wiley, New York, 1972), p. 294, Eq. (15.13).

[10]The reason is simply that (11) was derived in the past only for central potentials.