We consider scattering of a three-dimensional particle on a finite family of $\delta$ potentials. For some parameter values the scattering wavefunctions exhibit nodal lines in the form of closed loops, which may touch but do not entangle. The corresponding probability current forms vortical singularities around these lines; if the scattered particle is charged, this gives rise to magnetic flux loops. The conclusions extend to scattering on hard obstacles or smooth potentials.

The fact that quantum systems may exhibit nontrivial topological effects is known for long [1]. Recent interest to vortices has been focused mostly at superconducting systems described by the Ginzburg–Landau equation [2]. However, vortices have been also observed in pure quantum mechanics, specifically in numerical analysis of various models of mesoscopic electron transport [3] where they may arise even without an applied magnetic field.

The vortical behavior in quantum mechanical scattering is closely related with the wavefunction phase. Writing $\psi(\vec{r}) = \sqrt{\rho(\vec{r})} e^{i\phi(\vec{r})}$, we can express the probability current as $j(\vec{r}) = \rho(\vec{r}) \nabla \phi(\vec{r})$. In a region where external forces are absent, the integral of $j(\vec{r})$ over a closed loop can be nonzero only if it encircles a singularity in which the phase $\phi$ is ambiguous. However, solutions to the stationary Schrödinger equation are smooth functions, so only such singularities are zeros of $\psi$.

The existing results mentioned above are usually concerned with two-dimensional systems where the vortices are planar and centered around nodal points. The aim of the present letter is to show how the probability flow vortices look like in three dimensions, where nodal sets of the scattering wavefunctions are generically smooth curves. While the examples of Ref. [3] deal with perturbed channels of various shapes, the presence of the boundary is in fact not essential for the existence of vortical solutions. To illustrate this we shall discuss scattering in $\mathbb{R}^3$. For the sake of simplicity we are going to analyze a simple example of a particle scattered on a finite family of point interactions, however, the conclusions extend to a much wider family of potentials.

We shall demonstrate that scattering wavefunctions have often nodal lines, and that the latter are of the form of closed loops. The probability current in the vicinity of the line is locally cylindric (tornado-shaped). Moreover, if the scattered particles are charged, the corresponding electric current generates a magnetic field whose flux lines not far from the nodal lines are closed.

Let us describe the model. The point interactions will be treated in the standard way [3]. We suppose that they are finitely many and supported by a set $Y := \{ \vec{y}_j : j = 1, \ldots, N \}$. In the vicinity of the point $\vec{y}_j$ any solution to the stationary Schrödinger equation behaves as

$$\psi(\vec{x}) = \frac{A_j}{4\pi|\vec{x} - \vec{y}_j|} + B_j + \mathcal{O}(|\vec{x} - \vec{y}_j|),$$

where the coefficients are related by $B_j + \alpha_j A_j = 0$ and the real parameter $\alpha_j$ characterizes the interaction “strength” [3].

Suppose that the incident particle momentum is parallel to the first axis and equals $k$. For a given family of the coupling constants, $\alpha := \{\alpha_1, \ldots, \alpha_N\}$, the scattering wavefunction equals [3, Sec. II.1.5]

$$\psi_{\alpha,Y}(k; \vec{x}) = e^{ikx} + \sum_{j,\ell=1}^N [\Gamma_{\alpha,Y}(k)]_{j\ell}^{-1} e^{iky_{j\ell}} e^{ik|\vec{x} - \vec{y}_j|}$$

where $\Gamma_{\alpha,Y}(k) := \left[ \left( \frac{\alpha - ik}{4\pi} \right)^2 \delta_{j\ell} - G_k(\vec{y}_j - \vec{y}_\ell) \right]_{j,\ell=1}^N$, $\alpha := \{\alpha_1, \ldots, \alpha_N\}$, $\Gamma_{\alpha,Y}(k)$ denotes the Green’s function,

$$\Gamma_{\alpha,Y}(k) := \left[ \left( \frac{\alpha - ik}{4\pi} \right)^2 \delta_{j\ell} - G_k(\vec{y}_j - \vec{y}_\ell) \right]_{j,\ell=1}^N,$$

for $|\vec{x}| \neq 0$ and zero otherwise. We denote by $\mathcal{R}$, $\mathcal{I}$ the real and imaginary part of the function $\psi_{\alpha,Y}(k; \cdot)$, respectively; to find nodal sets one has to solve the equations

$$\mathcal{R}(x, y, z) = 0 = \mathcal{I}(x, y, z).$$

Some conclusions about the existence and properties of the solutions can be derived from the implicit–function theorem [2].

(i) In the absence of the scatterers, solutions to each of the conditions (1) are planes perpendicular to
the \(x\)-axis. They can be used as “unperturbed” solutions, since
\[
\frac{\partial R}{\partial x} \left( \left( n + \frac{1}{2}\right) \pi, y, z \right) \neq 0, \quad \frac{\partial I}{\partial x} (n\pi, y, z) \neq 0
\]
as \(y^2 + z^2 \rightarrow \infty\). Hence far enough from the scatterers the solutions to the two conditions are locally unique.

(ii) Whenever a unique solution exists, it is locally a \(C^\infty\) surface, since \(R, I\) are real-analytic functions of the variables \(x, y, z\). For the same reason, the sought nodal sets are \(C^\infty\) curves being intersections of two surfaces, except for possible crossing points where the solution is locally nonunique.

(iii) The implicit-function theorem also implies that the nodal lines are confined to a bounded region of the configuration space only. Indeed, the zero surfaces are for large \(y^2 + z^2\) of the form
\[
x_1 = \left( n + \frac{1}{2}\right) \pi + f_n(y, z), \quad x_1 = n\pi + g_n(y, z),
\]
respectively, and the smooth functions \(f_n, g_n\) are \(O((y^2 + z^2)^{-1/2})\), so that there is no intersection for \(y^2 + z^2\) large enough; for large \(|n|\) the argument can be extended up to the \(x\)-axis.

Before we shall discuss whether the solutions do exist, let us point out two other properties:

(iv) It follows from (iii) that the nodal line, if they exist, consist of a family of closed loops, each of them being a \(C^\infty\) curve. They can cross; this happens if one of the surfaces has locally a saddle shape and the other one — appropriately shifted by parameter choice — is “flatter”, i.e., has a small enough mean curvature.

(v) On the other hand, the loops cannot entangle into nontrivial knots, because any closed loop on a smooth surface without intersections is topologically equivalent to a circle; one cannot “draw” a knot upon a surface.

Before proceeding further, let us remark that the above argument has two basic ingredients. One is the finite range of the interaction which implies that far from the scattering centers the zero surfaces of the functions \(R\) and \(I\) cannot intersect. The other is the analyticity of the wavefunction with respect to the coordinates. Since this property persists if point scatterers are replaced by finite hard obstacles or a smooth enough potential, the conclusions are expected to apply to a much wider class of three-dimensional scattering systems.

To show that the described scheme is not empty, let us discuss next the case of a single \(\delta\) potential of the “strength” \(\alpha\) situated at the origin. In view of the cylindrical symmetry, possible nodal lines are circular loops perpendicular to the \(x\)-axis, hence we replace \((y, z)\) by \((y \cos \varphi, y \sin \varphi)\) so \(|\vec{x}| = \sqrt{x^2 + y^2}\). The scattering solution \((\psi)\) now acquires the form
\[
\psi_{\alpha,0}(k; \vec{x}) = e^{ikx} + \frac{e^{ik|x|}}{4\pi - ik|x|},
\]
where the right side turns to zero if
\[
eq 4\pi - \alpha.
\]
Taking the modulus, we find the distance of the ring from the origin,
\[
|x| = \frac{1}{\sqrt{k^2 + 16\pi^2\alpha^2}}.
\]
Furthermore, comparing the real and imaginary part in \(\psi\) we find
\[
|x| - x = -\frac{1}{k} \arctan \frac{k}{4\pi\alpha},
\]
where the arctangent branch remains to specified. Denoting the right side of \(\psi\) as \(-\gamma\) and substituting into \(|\vec{x}| = x^2 + y^2\), we get
\[
y^2 = \gamma^2 - 2\gamma x = -\gamma(\gamma + 2|x|).
\]
A nontrivial nodal ring exists if the left side is positive. It is straightforward to see from here that this happens if \(-2|x| < \gamma < 0\); introducing \(\kappa := k/4\pi\alpha\) we can rewrite the last condition as
\[
-\frac{2|\kappa|}{\sqrt{1 + \kappa^2}} < \arctan \kappa < 0.
\]
At the edges of the interval the ring shrinks into a nodal point. Inspecting the inequalities \((11)\), we infer that for \(\alpha < 0\) there is a unique solution given by the basic branch. On the other hand, one has to use arctan \(\kappa = n\pi\) if \(\alpha > 0\) and the solution exists provided \(\kappa > 2.971\), i.e.
\[
\frac{\alpha}{k} < 2.679 \times 10^{-2}.
\]
If there is more than one point scatterer, it is no longer possible to find the nodal lines analytically. However, the explicit form \((\psi)\) of the scattering wavefunction allows a numerical treatment. This demonstrates not only that the nodal loops can exist in the multicenter situation too, but also their possible crossing described in point (v) above; changing appropriately the parameters, one can achieve that a loop undergoes a fission process in which it is first “strangled” and then decays into two loops. As an illustration we show in Fig. 1. nodal lines inside a given rectangular “box” corresponding to 10 scattering centers whose positions are marked by dots. All the point interactions have the same strength \(\alpha = 0\). To convey the their spatial shapes, we do not plot the lines themselves
but rather their properly lighted tubular neighborhoods of radius $R = 0.1$.

To understand the behavior of the wavefunction in the vicinity of the nodal lines, one has to realize that due to the smoothness of the latter, the wavefunction has locally an approximate cylindrical symmetry. Hence if we want to expand $\psi_{\alpha,Y}(k;\vec{r})$, it is natural to place the point of interest into the origin with the nodal line tangent to the $z$ axis, we can use again the coordinates of the above example and write

$$\psi_{\alpha,Y}(k;\vec{r}) = \sum_{m \neq 0} c_m e^{im\varphi} J_m(ky).$$

The $m = 0$ term is missing because the wavefunction vanishes by assumption at $y = 0$. The phase behavior around the node is determined by the terms with the lowest nonzero $|m|$. Suppose that $c_1$ or $c_{-1}$ is nonzero and $|c_1| \neq |c_{-1}|$. Up to higher–order terms, the probability current $\vec{j}(\vec{r})$ is then located in a plane perpendicular to the nodal line and

$$\int_C \vec{v}(\vec{r}) \, d\vec{r} = \frac{2\pi}{\hbar} sgn(|c_1| - |c_{-1}|) ;$$

where $\vec{v}$ denotes the velocity of the probability flow, $\vec{v}(\vec{r}) := \nabla \phi(\vec{r})$. By analyticity this result extends to any curve $C$ encircling the nodal line once as long as it stays away of the scattering centers. It is moreover clear that the described case is generic, because it corresponds to simple zeros of the wavefunction. Higher winding numbers may appear only if there is $m_0 > 0$ such that $c_m = 0$ for $m = -m_0, -m_0 + 1, \ldots, m_0$.

To illustrate these considerations we choose a part of the “lowest” nodal loop of Fig. 1. To show that this is indeed the $|m| = 1$ case, we plot in Fig. 2 the wavefunction phase modulo $2\pi$ in the planes perpendicular to the loop. A single cut is clearly visible. In Fig. 3 we plot currents vectors at a tubular surface centered at the nodal line.

Let us ask whether the existence of “tornados” can have observable consequences. We have remarked that scattering of charged particles may produce in this way closed magnetic flux lines. Consider therefore a scattering of electrons and heavy ions in the presence of fixed obstacles. If the ion–obstacle configuration is properly chosen, the electrons should exhibit interference behavior of the AB type.

In conclusion, we have shown here analytically and demonstrated numerically that the probability flux in three–dimensional scattering can exhibit vortical behavior around nodal lines of the wavefunction. The latter are generically closed smooth curves which may intersect but do not entangle into knots, with the probability current velocity integral over a curve encircling the nodal line once equal to $\pm 2\pi$.

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Figure captions

Figure 1. Nodal lines of the wavefunction (shown by means of their lighted tubular neighborhoods) for scattering on $10 \delta$ potentials of the same strength $\alpha = 0$, whose positions are marked by dots, with the incident particle momentum $k = 2$.

Figure 2. Wavefunction phase around the “lowest” loop of the preceding picture. The wavefunction phase $\phi(\vec{r})$ has been evaluated mod $2\pi$ on a tubular surface of radius 0.1 along the nodal line and plotted in the perpendicular planes being scaled down by the factor 0.02.
Figure 3. The probability flow at the same tubular surface as in Fig. 2, the observation point is changed.
