17
The Schrödinger field

The Schrödinger equation is the quantum mechanical representation of the non-relativistic energy equation

$$\frac{\mathbf{p}^2}{2m} + V = E \tag{17.1}$$

and is obtained by making the replacement $p_i \rightarrow -\mathrm{i}\hbar\partial_i$ and $E = \mathrm{i}\hbar\tilde{\partial}_t$, and allowing the equation to operate on a complex field $\psi(x)$. The result is the basic equation of quantum mechanics

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = \mathrm{i}\hbar\tilde{\partial}_t\psi. \tag{17.2}$$

which may also be written

$$H_{\mathrm{D}}\psi = \mathrm{i}\hbar\tilde{\partial}_t\psi, \tag{17.3}$$

thereby defining the differential Hamiltonian operator. The free Hamiltonian operator H_0 is defined to be the above with $V = 0$.

17.1 The action

The action for the Schrödinger field is

$$S = \int \mathrm{d}\sigma\,\mathrm{d}t \Big\{ -\frac{\hbar^2}{2m}(\partial^i\psi)^*(\partial_i\psi) - V\psi^*\psi + \frac{\mathrm{i}\hbar}{2}(\psi^*\tilde{\partial}_t\psi - \psi\tilde{\partial}_t\psi^*) - J^*\psi - \psi^* J \Big\}. \tag{17.4}$$

Notice that this is not Lorentz-invariant, and cannot be expressed in terms of $n+1$ spacetime dimensional vectors.

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17.2 Field equations and continuity

The variation of the action can be performed with respect to both $\psi(x)$ and $\psi^*(x)$ since these are independent variables. The results are

$$\delta_{\psi^*} S = \int \mathrm{d}\sigma \mathrm{d}t \;\; \delta\psi^* \left(\frac{\hbar^2}{2m} \partial^i \partial_i \psi - V\psi + \mathrm{i}\hbar \tilde{\partial}_t \psi \right)$$

$$+ \int \mathrm{d}\sigma \left[\frac{\mathrm{i}\hbar}{2} \delta\psi^* \psi \right] + \int \mathrm{d}\sigma^i \left[\frac{\hbar^2}{2m} \delta\psi (\partial_i \psi)^\dagger \right] = 0$$

$$\delta_{\psi} S = \int \mathrm{d}\sigma \mathrm{d}t \;\; \delta\psi \left(\frac{\hbar^2}{2m} \partial^i \partial_i \psi^* - V\psi^* - \mathrm{i}\hbar \tilde{\partial}_t \psi^* \right)$$

$$+ \int \mathrm{d}\sigma \left[-\frac{\mathrm{i}\hbar}{2} \delta\psi \psi^* \right] + \int \mathrm{d}\sigma^i \left[\frac{\hbar^2}{2m} \delta\psi^* (\partial_i \psi) \right] = 0, \qquad (17.5)$$

where we have used integration by parts, and the two expressions are mutually conjugate. From the surface terms, we can now infer that the canonical momentum conjugate to $\psi(x)$ is

$$\Pi = \mathrm{i}\hbar\psi, \qquad (17.6)$$

and that spatial continuity at an interface is guaranteed by the condition

$$\Delta \left(\frac{\hbar^2}{2m} (\partial_i \psi) \right) = 0, \qquad (17.7)$$

where Δ means the change in value across the interface.

17.3 Free-field solutions

The free-field solutions may be written in a compact form as a linear combination of plane waves satisfying the energy constraint:

$$\psi(x) = \int_0^\infty \frac{\mathrm{d}\tilde{\omega}}{2\pi} \int_{-\infty}^{+\infty} \frac{\mathrm{d}^n \mathbf{k}}{(2\pi)^n} \mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\Delta\mathbf{x} - \tilde{\omega}\Delta t)} \; \psi(\mathbf{k}, \tilde{\omega})$$

$$\times\; \theta(\tilde{\omega}) \; \delta\left(\frac{\hbar^2 \mathbf{k}^2}{2m} - \hbar\tilde{\omega} \right). \qquad (17.8)$$

The coefficients of the Fourier expansion $\psi(\mathbf{k}, \tilde{\omega})$ are arbitrary.

17.4 Expression for the Green function

The Schrödinger Green function contains purely retarded solutions. This is a consequence of its spectrum of purely positive energy solutions. If one views the Schrödinger field as the non-relativistic limit of a relativistic field, then the

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negative frequency Wightman function for the relativistic field vanishes in the non-relativistic limit as a result of choosing only positive energy solutions. The Fourier space expression for the free-field Green function is

$$G_{\rm NR}(x,x') = \int_{-\infty}^{+\infty} \mathrm{d}\tilde{\omega} \int_{-\infty}^{+\infty} \frac{\mathrm{d}^n \mathbf{k}}{(2\pi)^n} \frac{\mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\Delta\mathbf{x}-\tilde{\omega}\Delta t)}}{(\frac{\hbar^2\mathbf{k}^2}{2m}-\hbar\tilde{\omega})-\mathrm{i}\epsilon}. \tag{17.9}$$

This may be interpreted in the light of the more general expression:

$$\begin{aligned} G_{\rm NR}(x,x') &= \sum_n \theta(t-t')\, u_n(x)u_n^*(x') \\ &= \int \frac{\mathrm{d}\alpha}{2\pi} \mathrm{e}^{-\mathrm{i}\alpha(t-t')} \frac{u_n(x)u_n^*(x')}{\alpha-\omega_n+\mathrm{i}\epsilon} \end{aligned} \tag{17.10}$$

where $u_n(x)$ are a complete set of eigenfunctions of the free Hamiltonian, i.e.

$$(H_0 - E_n)u_n(x) = 0, \tag{17.11}$$

where $E_n = \hbar\omega_n$.

17.5 Formal solution by Green functions

The free Schrödinger Green function satisfies the equation

$$\left(-\frac{\hbar^2\nabla^2}{2m} - \mathrm{i}\hbar\tilde{\partial}_t\right) G_{\rm NR}(x,x') = \delta(\mathbf{x},\mathbf{x}')\delta(t,t'), \tag{17.12}$$

or

$$(H_0 - E)G_{\rm NR}(x,x') = \delta(\mathbf{x},\mathbf{x}')\delta(t,t'), \tag{17.13}$$

and provides the solution for the field perturbed by source $J(x)$,

$$\psi(x) = \int (\mathrm{d}x')G_{\rm NR}(x,x')J(x'). \tag{17.14}$$

The infinitesimal source J is not normally written as such, but rather in the framework of the potential V, so that $J = V\psi$:

$$(H_0 - E_n)\psi_n = -V\psi_n, \tag{17.15}$$

where $\psi(x) = \sum_n c_n\psi_n(x)$. Substitution of this into the above relation leads to an infinite regression:

$$\begin{aligned} \psi(x) &= \int (\mathrm{d}x')G_{\rm NR}(x,x')J(x') \\ &= \int (\mathrm{d}x')G_{\rm NR}(x,x')V(x')\psi(x') \\ &= \int (\mathrm{d}x')(\mathrm{d}x'')G_{\rm NR}(x,x')G_{\rm NR}(x',x'')J(x''), \end{aligned} \tag{17.16}$$

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and so on. This multiplicative hierarchy is only useful if it converges. It is thus useful to make this into an additive series, which converges for sufficiently weak $V(x)$. To do this, one defines the free-field $\psi_0(x)$ as the solution of the free-field equation

$$(H_0 - E_n)\psi_{0n}(x) = 0, \tag{17.17}$$

and expands in the manner of a perturbation series. The solutions to the full-field equation are defined by

$$\psi_n(x) = \psi_{0n}(x) + \delta\psi_n \tag{17.18}$$

where the latter terms are assumed to be small in the sense that they lead to convergent results in calculations. Substituting this into eqn. (17.15) gives

$$(H_0 - E_n)\delta\psi_n = -V(x)\psi_n(x), \tag{17.19}$$

and thus

$$\delta\psi(x) = -\int (\mathrm{d}x')\; G_{\mathrm{NR}}(x, x')\, V(x')\psi(x'), \tag{17.20}$$

or

$$\psi(x) = \psi_0(x) - \int (\mathrm{d}x')\; G_{\mathrm{NR}}(x, x')\, V(x')\psi(x'). \tag{17.21}$$

This result is sometimes called the *Lippmann–Schwinger equation*. The equation can be solved iteratively by re-substitution, i.e.

$$\begin{aligned}\psi(x) = \psi_0(x) &- \int (\mathrm{d}x')\; G_{\mathrm{NR}}(x, x')\, V(x')\psi_0(x'') \\ &+ \int (\mathrm{d}x')(\mathrm{d}x'')\; G_{\mathrm{NR}}(x, x')G_{\mathrm{NR}}(x', x'')\, V(x')V(x'')\psi_(x''),\end{aligned} \tag{17.22}$$

and generates the usual quantum mechanical perturbation series, expressed in the form of Green functions.

17.6 Conserved norm and probability

The variation of the action with respect to constant δs under a phase transformation $\psi \to \mathrm{e}^{\mathrm{i}s}\psi$ is given by

$$\begin{aligned}\delta S = \int (\mathrm{d}x)\Bigg\{ &- \frac{\hbar^2}{2m}\left[-\mathrm{i}\delta s(\partial^i\psi^*)(\partial_i\psi) + (\partial^i\psi^*)\mathrm{i}\delta s(\partial_i\psi)\right] \\ &+ \mathrm{i}\left[-\mathrm{i}\delta s\,\psi^*\tilde{\partial}_t\psi + \mathrm{i}\delta s\,\psi^*\tilde{\partial}_t\psi\right]\Bigg\}.\end{aligned} \tag{17.23}$$

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Integrating by parts and using the equation of motion, we obtain the expression for the continuity equation,

$$\delta S = \int (\mathrm{d}x)\delta s \left(\tilde{\partial}_t J^t + \partial_i J^i\right) = 0, \tag{17.24}$$

where

$$\begin{aligned} J^t &= \psi^* \psi = \rho \\ J^i &= \frac{\mathrm{i}\hbar^2}{2m}\left[\psi^*(\partial^i \psi) - (\partial^i \psi^*)\psi\right], \end{aligned} \tag{17.25}$$

which can be compared to the current conservation equation eqn. (12.1). ρ is the probability density and J^i is the probability current. The conserved probability is therefore

$$P = \int \mathrm{d}\sigma\, \psi^*(x)\psi(x), \tag{17.26}$$

and this can be used to define the notion of an inner product between two wavefunctions, given by the overlap integral

$$(\psi_1, \psi_2) = \int \mathrm{d}\sigma\, \psi_1^*(x)\psi_2(x). \tag{17.27}$$

17.7 Energy–momentum tensor

Replacing $\eta_{\mu\nu}$ by $\delta_{\mu\nu}$ (the Euclidean metric), we have for the components of the energy–momentum tensor:

$$\begin{aligned} \theta_{tt} &= \frac{\partial \mathcal{L}}{\partial(\tilde{\partial}_t \psi)}(\tilde{\partial}_t \psi) + (\tilde{\partial}_t \psi^*)\frac{\partial \mathcal{L}}{\partial(\tilde{\partial}_t \psi)^*} - \mathcal{L} \\ &= \frac{\hbar^2}{2m}(\partial^i \psi)^\dagger(\partial_i \psi) + V\psi^*\psi, \qquad (17.28) \\ &\equiv H. \qquad (17.29) \end{aligned}$$

In the second-quantized theory, where $\psi(x)$ is a field operator, this quantity is often called the Hamiltonian density operator H. This is to be distinguished from H_{D}, the differential Hamiltonian operator. In the classical case, the spatial integral of θ_{tt} is the expectation value of the Hamiltonian, as may be seen by integration by parts:

$$\begin{aligned} H = \int \mathrm{d}\sigma \theta_{tt} &= \int \mathrm{d}\sigma\ \psi(x)^* \left[-\frac{\hbar^2}{2m}\partial^2 + V\right]\psi(x) \\ &= (\psi, H_{\mathrm{D}}\psi) \\ &\equiv \langle H_{\mathrm{D}} \rangle. \end{aligned} \tag{17.30}$$

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Thus, θ_{tt} represents the total energy of the fields in the action S. The off-diagonal spacetime components are related to the expectation value of the momentum operator

$$\begin{aligned}\theta_{ti} &= \frac{\partial \mathcal{L}}{\partial \tilde{\partial}_t \psi}(\partial_i \psi) + (\partial_i \psi^*)\frac{\partial \mathcal{L}}{\partial \tilde{\partial}_t \psi^*} = \frac{\mathrm{i}\hbar}{2}\psi^*(\partial_i \psi) - \frac{\mathrm{i}\hbar}{2}(\partial_i \psi^*)\psi \\ \int \mathrm{d}\sigma\, \theta_{ti} &= (\psi, \mathrm{i}\hbar \partial_i \psi) \\ &= -\langle p_i \rangle,\end{aligned} \tag{17.31}$$

and

$$\begin{aligned}\theta_{it} &= \frac{\partial \mathcal{L}}{\partial(\partial_i \psi)}(\tilde{\partial}_t \psi) + \frac{\partial \mathcal{L}}{\partial(\partial_i \psi^*)}(\tilde{\partial}_t \psi^*) \\ &= -\frac{\hbar^2}{2m}\left\{(\partial_i \psi)^*(\tilde{\partial}_t \psi) + (\partial_i \psi)(\tilde{\partial}_t \psi)^*\right\}.\end{aligned} \tag{17.32}$$

Note that θ is not symmetrical in the spacetime components: $\theta_{it} \neq \theta_{ti}$. This is a result of the lack of Lorentz invariance. Moreover, the sign of the momentum component is reversed, as compared with the relativistic cases, owing to the difference in metric signature. Finally, the 'stress' in the field is given by the spatial components:

$$\begin{aligned}\theta_{ij} &= \frac{\partial \mathcal{L}}{\partial(\partial_i \psi)}(\partial_j \psi) + \frac{\partial \mathcal{L}}{\partial(\partial_i \psi)^*}(\partial_j \psi)^* - \mathcal{L}\delta_{ij} \\ &= -\frac{\hbar^2}{2m}\left\{(\partial_i \psi)^*(\partial_j \psi) + (\partial_i \psi)(\partial_j \psi)^* - (\partial^k \psi)^*(\partial_k \psi)\delta_{ij}\right\} \\ &+ \left\{V\psi^*\psi - \frac{\mathrm{i}\hbar}{2}(\psi^* \overset{\leftrightarrow}{\tilde{\partial}_t} \psi)\right\}\delta_{ij}.\end{aligned} \tag{17.33}$$

Using the field equation (17.2), the trace of the spatial part may be written

$$\begin{aligned}\mathrm{Tr}\,\theta_{ii} &= (n-2)\frac{\hbar^2}{2m}(\partial^k \psi)^*(\partial_k \psi) + n\left(V\psi^*\psi - \frac{1}{2}\frac{\hbar^2}{2m}\psi^* \overset{\leftrightarrow}{\partial^2} \psi\right) \\ &= (1-n)\,H + 2V\psi^*\psi,\end{aligned} \tag{17.34}$$

where the last line is obtained by partial integration over all space, and on identifying the first and last terms as being $H - V$, and is therefore true only up to a partial derivative, or under the integral sign. See also Jackiw and Pi for a discussion of a conformally improved energy–momentum tensor, coupled to electromagnetism [78].

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