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Short note: Hamiltonian for a particle with position-dependent mass

J. R. Morris

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Abstract An approach for obtaining a Schrödinger equation for a spinless nonrelativistic particle with a position-dependent mass is proposed. Rather than starting with the nonrelativistic hamiltonian for a free particle, we begin with its relativistic completion in the form of a Klein–Gordon equation and then reduce it to obtain the nonrelativistic limit. This type of procedure avoids the usual ordering ambiguities that commonly arise in obtaining a Schrödinger equation for a particle with position-dependent mass.

Keywords Position-dependent mass · Hamiltonian · Schrödinger equation

1 Introduction

Various ideas and approaches exist for generating a hamiltonian for a particle with a position-dependent mass $m(\boldsymbol{x})$ [1–7]. These approaches typically involve writing a classical particle lagrangian with a kinetic term $\frac{1}{2}m(\boldsymbol{x})\boldsymbol{u}\cdot\boldsymbol{u} = \frac{1}{2}\boldsymbol{p}\cdot\boldsymbol{p}/m(\boldsymbol{x})$ and then introducing a canonical quantization prescription where $\boldsymbol{p} \to -i\hbar\nabla$ is used. However, there is an ordering ambiguity that arises due to the mass $m(\boldsymbol{x})$. The ambiguity results in different possible quantum hamiltonians, which, in general, are not equivalent (see, for example, [3,5,7]). A few examples of inequivalent forms of the quantum kinetic energy operator are (see [7] and references therein) as follows:

$$\hat{T} = -\frac{1}{4}\left(m^{-1}\nabla^2 + \nabla^2 m^{-1}\right)$$

$$\hat{T} = -\frac{1}{2}\nabla m^{-1}\nabla$$

$$\hat{T} = -\frac{1}{2}\left(\sqrt{m^{-1}}\nabla^2\sqrt{m^{-1}}\right)$$

$$\hat{T} = -\frac{1}{4}\left(m^{-1}\right)^{\alpha}\nabla(m^{-1})^{\beta}\nabla(m^{-1})^{\gamma} + H.c.$$

with $\alpha + \beta + \gamma = 1$.

Here, a different type of procedure is proposed which avoids these ambiguities. Rather than starting with the nonrelativistic classical kinetic energy $E = \frac{1}{2}m(\boldsymbol{x})\boldsymbol{u}\cdot\boldsymbol{u} = \frac{1}{2}\boldsymbol{p}\cdot\boldsymbol{p}/m(\boldsymbol{x})$ and proceeding with quantization, we

J. R. Morris (✉)
Department of Physics, Indiana University Northwest, 3400 Broadway, Gary, IN 46408, USA
e-mail: jmorris@iun.edu

begin using the relativistic extension for a spinless "free" boson obeying $p_\mu p^\mu - m^2(\boldsymbol{x}) = 0$, i.e., $E^2 - \boldsymbol{p}^2 - m^2(\boldsymbol{x}) = 0$. Here, we use a flat spacetime metric with signature $(+,-,-,-)$ and natural units with $\hbar = c = 1$. We also note that a position dependence of the mass can arise from different types of interactions; see [8–11] and references therein. The quantization prescription $p_\mu \to i\partial_\mu$, i.e., $\boldsymbol{p} \to -i\nabla$, $E \to i\partial_t$, then yields a Klein–Gordon equation $\Box\phi + m^2(\boldsymbol{x})\phi = 0$ for a complex-valued boson field $\phi(x^\mu)$, where $\Box = \partial_t^2 - \nabla^2$. A reduction to the nonrelativistic limit will then yield a Schrödinger equation for the position-dependent mass, without the ordering ambiguities.

We presently specialize to the case where the mass $m(\boldsymbol{x})$ is a mildly varying function which can be characterized by a constant mass parameter m_0 with $m(\boldsymbol{x}) = m_0 + \delta m(\boldsymbol{x}) = \mu(\boldsymbol{x})m_0$, where $\mu = m/m_0$ and $|\delta m/m_0| \ll 1$, so that $m(\boldsymbol{x})$ never wanders far from the characteristic mass m_0. A Klein–Gordon equation $\Box\phi + m_0^2\phi$ for a field with constant mass m_0 can be reduced to a Schrödinger equation form using a technique illustrated by Bjorken and Drell [12], or by one that has been introduced by Adler and Chen [13]. Here, we employ the Adler–Chen method for its relative simplicity, and apply this to the case where the mass is position-dependent, with $|\delta m| \ll m_0$.

2 Schrödinger equation

Constant mass We begin with the Klein–Gordon equation for a complex scalar field:

$$\ddot{\phi} - \nabla^2\phi + m^2(\boldsymbol{x})\phi = 0 \tag{1}$$

where $m(\boldsymbol{x}) = m_0 + \delta m(\boldsymbol{x}) = \mu(\boldsymbol{x})m_0$, and $|\delta m/m_0| \ll 1$. We can also write $\mu = m/m_0 = 1 + \delta m/m_0$. We now split out the rapid time variation of ϕ due to the rest mass by writing

$$\phi(\boldsymbol{x}, t) = e^{-im_0 t}\psi(\boldsymbol{x}, t). \tag{2}$$

Now, in the limit that the mass variation vanishes, $\delta m \to 0$, insertion of (2) into (1) yields

$$-\frac{1}{2m_0}\nabla^2\psi = i\dot{\psi} - \frac{1}{2m_0}\ddot{\psi}. \tag{3}$$

This looks like the Schrödinger equation for a free particle, except with the extra term $\ddot{\psi}/2m_0$, and is, therefore, referred to as the Schrödinger equation form, or SEF, by Adler and Chen [13]. This equation has an exact solution $\psi = \exp(-iEt + i\mathbf{p}\cdot\mathbf{x})$, where $E = E_{\text{rel}} - m_0$ is the nonrelativistic energy, i.e., the relativistic energy of the free particle with the rest energy subtracted off. In the low-energy limit, the $\ddot{\psi}/2m_0$ term becomes negligible in comparison to the $i\dot{\psi}$ term. If the $\ddot{\psi}$ term is dropped, we have the ordinary Schrödinger equation for a free nonrelativistic particle. In this limit, we have an approximate quantum mechanical description for a single free particle.

Let us look further at the probability interpretation for the wave function ψ. The (normalized) current density $j^\mu = \frac{i}{2m_0}\phi^* \overleftrightarrow{\partial^\mu} \phi$ for the Klein–Gordon field is conserved, $\nabla_\mu j^\mu = 0$. We use the notation $\phi^* \overleftrightarrow{\partial^\mu} \phi = \phi^*\partial^\mu\phi - (\partial^\mu\phi^*)\phi$ and $\partial^0 = \partial_0 = \partial_t$, $\partial^k = -\partial_k$. Now, using (2), we have

$$\begin{aligned} j^0 &= \psi^*\psi + \frac{i}{2m_0}\psi^* \overleftrightarrow{\partial^0} \psi \\ j^k &= \frac{i}{2m_0}\psi^* \overleftrightarrow{\partial^k} \psi. \end{aligned} \tag{4}$$

The current density component j^0 contains the extra term $\frac{i}{2m_0}\psi^* \overleftrightarrow{\partial^0} \psi$, so that the charge density j^0 does not coincide with the Schrödinger probability density $\rho = \psi^*\psi$. However, in the low-energy limit $E/m_0 \ll 1$, dropping this extra term leaves us with $j^0 = \rho = \psi^*\psi$. Therefore, in the low-energy limit $E \ll m_0$, we have the Schrödinger equation with the usual probability density and the nonrelativistic single particle quantum mechanical interpretation. This interpretation breaks down near an energy scale $E_{\text{viol}} \lesssim m_0$, and we must then use the UV completion, i.e., the Klein–Gordon equation, but for $E \ll E_{\text{viol}} \lesssim m_0$, the Schrödinger equation is valid. Relativistic corrections can then be computed with standard quantum mechanical perturbation theory, as long as we stay in an energy domain where $E \ll E_{\text{viol}} \lesssim m_0$.

Position-dependent mass For $\delta m \neq 0$ but $|\delta m|/m_0 \ll 1$, we expect the above to follow through with only minor modification. We again insert (2) into (1) to obtain

$$-\frac{1}{2m_0}\nabla^2\psi + \frac{m_0}{2}(\mu^2 - 1)\psi = i\dot{\psi} - \frac{1}{2m_0}\ddot{\psi}. \tag{5}$$

We again restrict ourselves to nonrelativistic energies $E \ll m_0$ and drop the $\ddot{\psi}/2m_0$ term. The result is a Schrödinger equation for a particle with mass m_0 with a potential

$$V(\boldsymbol{x}) = \frac{m_0}{2}(\mu^2 - 1) = \delta m(\boldsymbol{x}) \tag{6}$$

where we have used $\mu^2 = (1 + \delta m/m_0)^2 = 1 + 2\delta m/m_0$. We, therefore, have an effective Schrödinger equation for a wave function $\psi(\boldsymbol{x}, t)$ given by the following:

$$-\frac{1}{2m_0}\nabla^2\psi + \delta m(\boldsymbol{x})\psi = i\dot{\psi} \tag{7}$$

valid for energies $E \ll m \approx m_0$.

Probability and current densities The lagrangian for the Klein–Gordon field ϕ with position-dependent mass $m(\boldsymbol{x})$ is as follows:

$$\mathcal{L} = \partial_\mu\phi^*\partial^\mu\phi - m^2\phi^*\phi \tag{8}$$

which yields the equation of motion (1). We now wish to obtain the conserved current density J^μ for this system and check the probability interpretation in the low-energy limit. The lagrangian $\mathcal{L}$ is invariant under a global phase transformation:

$$\begin{aligned} \phi &\to e^{i\alpha}\phi = (1 + i\alpha)\phi \\ \phi^* &\to e^{-i\alpha}\phi^* = (1 - i\alpha)\phi^* \end{aligned} \tag{9}$$

where $\alpha =$ const and we consider the infinitesimal transformation with

$$\delta\phi = i\alpha\phi, \ \ \delta\phi^* = -i\alpha\phi^*. \tag{10}$$

Under these transformations, $\delta\mathcal{L} = 0$, and the Noether procedure provides a conserved current:

$$\begin{aligned} \delta\mathcal{L} &= \frac{\partial\mathcal{L}}{\partial\phi}\delta\phi + \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\delta(\partial_\mu\phi) + \left(\phi \to \phi^*\right) \\ &= \left[\frac{\partial\mathcal{L}}{\partial\phi} - \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\right)\right]\delta\phi \\ &\quad + \partial_\mu\left[\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\delta\phi\right] + \left(\phi \to \phi^*\right). \end{aligned} \tag{11}$$

The first term $\frac{\partial\mathcal{L}}{\partial\phi} - \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\right)$ on the right-hand side vanishes by the equation of motion for ϕ^*, and by (10), we have

$$i\alpha\partial_\mu\left[\frac{\partial\mathcal{L}}{\partial\left(\partial_\mu\phi\right)}\phi - \frac{\partial\mathcal{L}}{\partial\left(\partial_\mu\phi^*\right)}\phi^*\right] = 0 \tag{12}$$

so that by (8), we can identify a conserved Klein–Gordon current density

$$J^\mu = i\phi^*\overleftrightarrow{\partial^\mu}\phi \tag{13}$$

with $\nabla_\mu J^\mu = 0$. We then again employ (2) and multiply by the constant $1/2m_0$ to obtain the normalized probability and current densities $j^\mu = J^\mu/2m_0$ given by (4), which again, reduce to

$$j^0 = \rho = \psi^*\psi, \quad j^k = \frac{i}{2m_0}\psi^*\overleftrightarrow{\partial^k}\psi \tag{14}$$

in the low-energy limit $E \ll m_0$, i.e., the usual nonrelativistic quantum mechanical probability and current densities.

3 Discussion

A particle can obtain an effective position-dependent mass in different types of settings, for example in a condensed matter setting (see [7]) or in a setting involving gravitation with a conformal transformation of the action (see [8,9]). Starting with a nonrelativistic expression for the energy of a "free" particle $E = \boldsymbol{p}\cdot\boldsymbol{p}/2m(\boldsymbol{x})$ for a particle with a position-dependent mass, followed by a quantization using canonical replacements for energy and momentum operators, $\boldsymbol{p} \to -i\nabla$ and $E \to i\partial_t$, leads to ambiguities in the quantum hamiltonian, and can result in different, inequivalent hamiltonian operators and Schrödinger equations. This difficulty is sidestepped here with the proposition of starting with the relativistic quantum equation, the Klein–Gordon equation $\partial_t^2\phi - \nabla^2\phi + m^2(\boldsymbol{x})\phi = 0$ for a complex scalar field ϕ, and then taking the low-energy limit to obtain a Schrödinger equation. We have specialized to the case where there exists a constant mass parameter m_0 which serves to characterize the mass, with $\delta m = m - m_0 \ll m_0$, in other words, the mass is a mildly varying function of position. The result of this procedure is a Schrödinger equation, given by (7), for a particle with mass m_0 which contains a potential of the form $V(\boldsymbol{x}) = \frac{m_0}{2}(\mu^2 - 1) = \delta m(\boldsymbol{x})$ and is valid for energies $E \ll m_0$. The usual probability interpretation remains intact at low energy.

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