

Relativistic Correction to the Nonrelativistic Wavefunction

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In this note, we try to obtain a simple relativistic correction, using powers of $1/2$, to the nonrelativistic wavefunction using the one dimensional Dirac and Klein-Gordon equations, both with a scalar potential. A more accurate correction, including higher orders, can also be performed. (We find that due to cancellations and the removal of a $1/2m$ factor using the Schrodinger equation $-1/2m d/dx d/dx W_0 = (e-V) W_0$, second order terms $(1/2m)^2$ need to be kept.) We also try to apply this simple method to product wavefunctions $W(x)=W_0(x)W_1(x)$ where $W_0(x)$ is the ground state wavefunction to see how $W_1(x)$ is affected. It seems such a calculation may have already been performed in the literature, but we are unaware of any specific cases or any examples in textbooks, although in (1) an expansion in terms of v/c is performed.

Nonrelativistic Limit

The one dimensional Dirac equations:

$$-d/dx v(x) = (E-m_0-V) u(x) \quad ((1a)) \quad \text{and} \quad d/dx u(x) = (E+m_0+V) v(x) \quad ((1b))$$

may be converted into the Schrodinger equation as already shown in the literature. In particular: $E+m_0+V$ becomes $2m$ and $E-m_0-V$, $e-V$ where $e=E-m_0$ = the nonrelativistic energy. Thus, it seems $e-V$ and $e+V$ are considered small compared with m_0 in such an approach. We try to use this idea to obtain a simple relativistic correction to the nonrelativistic wavefunction. Small corrections to the three dimensional Dirac equations have been considered in (1), but using expansions in v/c . Using v/c as an expansion parameter is usual in nonrelativistic limits, but m_0 being large compared to e and $V(x)$ also appears frequently in the literature. We wish to base an expansion on the latter.

We begin with:

$u(x) = u_a(x) + u_b(x)$ where $u_b(x)$ is a lower order correction to $u_a(x)$. We use $1/2m$ and $e+V$ as small values. In such a case, ((1b)) is written as:

$$1/2m [1 - (e+V)/2m + (e+V)(e+V)/(2m)^2] (u_a + u_b) = v(x) \quad \text{and this is inserted into ((1a)) to give to:}$$

$$-1/2m d/dx d/dx u_a + (e+V)/2m d/dx d/dx u_a - 1/2m d/dx d/dx u_b + 1/2m (d/dx V) (d/dx u_a) + (d/dx d/dx u_a) (e+V)(e+V)/(2m)^3 = (e-V) (u_a+u_b) \quad ((2))$$

Now: $-1/2m d/dx d/dx u_a = (e-V)u_a$ (Schrodinger equation) so:

$$\begin{aligned} & (e+V)/2m \, d/dx \, d/dx \, u_a - 1/2m \, d/dx \, d/dx \, u_b + 1/2m \, (d/dx \, V) \, (d/dx \, u_a) - (d/dx \, d/dx \, u_a) \\ & (e+V)(e+V)/(2m)^3 = (e-V) \, u_b \quad ((3)) \end{aligned}$$

At this point, one has a second order DE in u_b to solve assuming u_a , the nonrelativistic solution is known. (It can be obtained by solving the Schrodinger equation.) If one uses the Klein-Gordon equation, one may be able to simplify this i.e.:

$$-d/dx \, d/dx \, (u_a + u_b) = [E^*E - (m_0 + V)^2] \, (u_a + u_b) \quad ((4))$$

$$E = m_0 + e \text{ so } [E^*E - (m_0 + V)^2] = e^*e + V^*V + 2m_0(e - v)$$

The last term is part of the Schrodinger equation: $-d/dx \, d/dx \, u_a = 2m(e - V) \, u_a$ so:

$$-d/dx \, d/dx \, u_b = (e^*e - V^*V) \, u_a + (e^*e - V^*V) \, u_b + 2m(e - V) \, u_b \quad ((4b)). \text{ Using } ((4b)) \text{ in } ((3)) \text{ yields:}$$

$$u(x) = u_a(x) + (1/(e^*e - V^*V)) \, 1/(2m) \, (d/dx \, V) \, (d/dx \, u_a) + (e+V)/2m \, u_a \quad ((5))$$

$$\text{So } u_b = (1/(e^*e - V^*V)) \, 1/(2m) \, (d/dx \, V) \, (d/dx \, u_a) + (e+V)/2m \, u_a$$

As a test, one should see if ((5)) satisfies ((4b)):

$$(e^*e - V^*V)u_a + 2m(e - V) \, u_b + (e^*e - V^*V) \, u_b - (e+V)/2m \, u_a = -d/dx \, d/dx \, u_b \quad ((5b))$$

The term $(e^*e - V^*V) \, u_b$ on the LHS may be dropped as it is small compared to the second term. If one examines ((5)), one sees there is a $1/2m$ term. This cancels the $2m$ of the second term of the LHS of ((5b)). Now:

$$d/dx \{ (1/(e^*e - V^*V)) \, (d/dx \, V) \, (d/dx \, u_a) \} \text{ yields a term proportional to } d/dx \, (d/dx \, d/dx \, u_a).$$

This in turn is proportional to $-2m(e - V) \, u_a$. Taking d/dx of this term (one initially has $-d/dx \, d/dx$) yields a term $(-2m)(e - V) \, d/dx \, u_a$. $d/dx \, d/dx$ operating on $(e+V)/2m \, u_a$ yields a term: $-(e+V)(e - V) \, u_a$ which cancels the first term on the LHS of ((5b)).

$$2m(e - V) \, u_b = -2m(e - v) \, (d/dx \, u_a) \text{ factor from } ((5))$$

The factor from ((5)) is $d/dx \, V \, 1/(e^*e - V^*V)$. Thus, the two sides are equal.

Other terms will have at least $1/2m$ and are of lower order.

We note, we have only kept some expansion terms in obtaining ((5)). One may obtain a more accurate correction. The coupling $(d/dx V) (d/dx u_a)$ is interesting because it is similar to $(d/dx u_0) (d/dx u_1)$ which is obtained if one writes the solution of the Schrodinger equation as $u(x)=u_0(x)u_1(x)$ where $u_0(x)$ is the ground state solution. In this case, $d/dx V(x)$ replaces $d/dx u_1$. It is almost as if the spatial flux (proportional to $d/dx u_a$) is coupling with $d/dx V$, a kind of flux of the potential if one writes the $V(x) = \text{Sum over } p V_p \exp(ipx)$. (V_p is the Fourier transform.)

Correction to $u(x)=u_0(x)u_1(x)$

Given the Schrodinger time independent equation, one may write the solution as: $u(x)=u_0(x)u_1(x)$ where $u_0(x)$ is the ground state solution. One may then ask what a relativistic correction to $u_1(x)$ would be. We start with ((5))

$$u_0 = u_{0a} + u_{0b} \text{ where } u_{0b} = (1/(e_0 * e_0 - V * V) - 1/(2m)) (d/dx V) (d/dx u_{0a}) + (e_0 + V)/2m u_{0a} \quad ((6))$$

$$\text{and } u = u_a + u_b \text{ where } u_b = (1/(e * e - V * V) - 1/(2m)) (d/dx V) (d/dx u_a) + (e + V)/2m u_a \quad ((7))$$

and $u_a = u_{0a} * u_{1a}$. Next:

$$u_1 = u_{1a} + u_{1b} \text{ and } u = u_a + u_b = (u_{0a} + u_{0b})(u_{1a} + u_{1b}) \quad ((8))$$

To first order:

$$u_b = u_{0a} u_{1b} + u_{0b} u_{1a} \quad ((9))$$

u_b , u_{0a} , and u_{1a} are known as u_{1a} is the solution of:

$$-1/2m d/dx d/dx u_{1a} - 1/m (d/dx u_{1a}) (d/dx u_{0a}/u_{0a}) = (e - e_0) u_{1a}$$

u_{0a} is the solution of the Schrodinger equation and u_{0b} is given by ((5)).

Thus, one can solve for u_{1b} which is the first order relativistic correction to u_1 . One finds:

$$u_{1b} = \{ + (1/(e * e - V * V) - 1/(2m)) (d/dx V) [d/dx (u_{1a} u_{0a})] + (e + V)/2m u_{0a} u_{1a} - u_{1a} \{ (1/(e_0 * e_0 - V * V) - 1/(2m)) (d/dx V) [d/dx (u_{0a})] + (e_0 + V)/2m u_{0a} \} \} / u_{0a} \quad ((10))$$

Conclusion

In conclusion, we have attempted to provide a simple (expansion in $1/2m$) relativistic correction to the Schrodinger wavefunction and the product wavefunction $W(x)=W_0(x)W_1(x)$ where $W_0(x)$ is the ground state wavefunction. Higher order, more accurate, corrections may be obtained by retaining terms dropped above.

References

1. Shankar, R. Principles of Quantum Mechanics (Plenum Press, 1988)